Safety, Health & Environment

ExxonMobil Chemical

ExxonMobil

Safety, Heath & Environment

Safety is our company's number one priority. We care for the safety of our employees and our customers. We care for the people who handle and use our products, for the communities living near facilities where these products are used and for our environment. The very strict risk management approach that we follow to maintain safety standards at their highest level is underpinned by the principle that "risk = hazard x exposure".
It indicates that an increase in the level of safety can be achieved by limiting exposure to hazardous substances and/or by using safer materials.

Physical hazards

Flammability is the only physical hazard associated with ExxonMobil Chemical fluids. It is not relevant to plasticizers, alcohols or neo acids, which are not classified as flammable as per current legislation. Volatile hydrocarbons and oxygenated fluids are used in a wide range of processes and equipment. Flammable by nature, they have to be used following strict guidelines to ensure safe operations.

Basics of flammability »

Guidelines for safe operations »

Basics of flammability

Fire is a very complex chemical process. The control of fire hazards and a safe environment requires a good understanding of the chemistry and physics of fire and the different ways to measure flammability. The flammability of fluids is measured from their physical properties and the conditions they have to meet for chemical reactions to take place.

Chemistry and physics of fire »

For a fire to start, 3 elements must combine: a flammable source, a source of ignition (e.g., heat) and an oxidant (i.e., oxygen).

Physical properties and flammability limits »

A number of properties are tested to measure the flammability limits of fluids. For example: vapor pressure, LEL and UEL, mists, vapor density.

Flash and fire points »

The flash point is the minimum temperature at which momentary combustion can happen. The fire point is the minimum temperature at which combustion can be sustained.

Auto ignition temperature »

The auto ignition temperature is the temperature at which a fluid will spontaneously ignite, without the presence of a source of ignition.

Ignitability and minimum ignition energy (MIE) »

MIE is the minimum amount of energy required to ignite a combustible vapor, gas or dust cloud, for example due to an electrostatic discharge.

Static electricity »

Among the sources of ignition which present a significant risk is static electricity. It builds up during the transfer of liquids especially hydrocarbon fluids.

Chemistry and physics of fire

For a fire to start, 3 elements must combine: a flammable source, a source of ignition (e.g., heat) and an oxidant (i.e., oxygen). A 4th element, called the chain reaction of combustion, is necessary to keep the fire alight.

Chemistry of combustion

Fire is a complex chemical process. It is therefore important to understand the basic principles relating to flammability:

- Flammability describes the ability of a substance to burn or combust with a flame.
- Combustion (or burning) describes an oxidation reaction between a fuel and an oxidant, accompanied by the production of heat and fire.

An example of combustion illustrated by a stoichiometric equation is the oxidation of a pure hydrocarbon such as **normal pentane**:

C_5H_{12} pentane fuel	+	$8\ O_2$ oxygen oxidant	→	$5\ CO_2$ carbon dioxide	+	$6\ H_2O$ water
Pentane burns in oxygen (air) to produce carbon dioxide and water with the release of heat. The heat of combustion of normal pentane is of about 49 Mega Joules per kg at 20°C.						

In the case of oxygenated solvents, such as isopropanol (IPA), the solvent contains not only carbon and hydrogen atoms but also oxygen. It can be considered that the oxygenated solvents are already somewhat oxidized and therefore their energy of combustion is lower than pure hydrocarbons:

$2CH_3\ (CH\text{-}OH)CH_3$ isopropanol fuel	+	$9\ O_2$ oxygen oxidant	→	$6\ CO_2$ carbon dioxide	+	$6\ H_2O$ water
The heat of combustion of isopropanol is significantly lower at 33 MJ/kg at 20°C.						

The fire triangle

For combustion to take place, both fuel and oxidant (most often oxygen) need to be present together with an ignition source of sufficient energy to initiate the reaction. The fire triangle provides a simple means to describe the three components necessary to generate a fire:

- flammable fluid
- oxygen
- source of ignition

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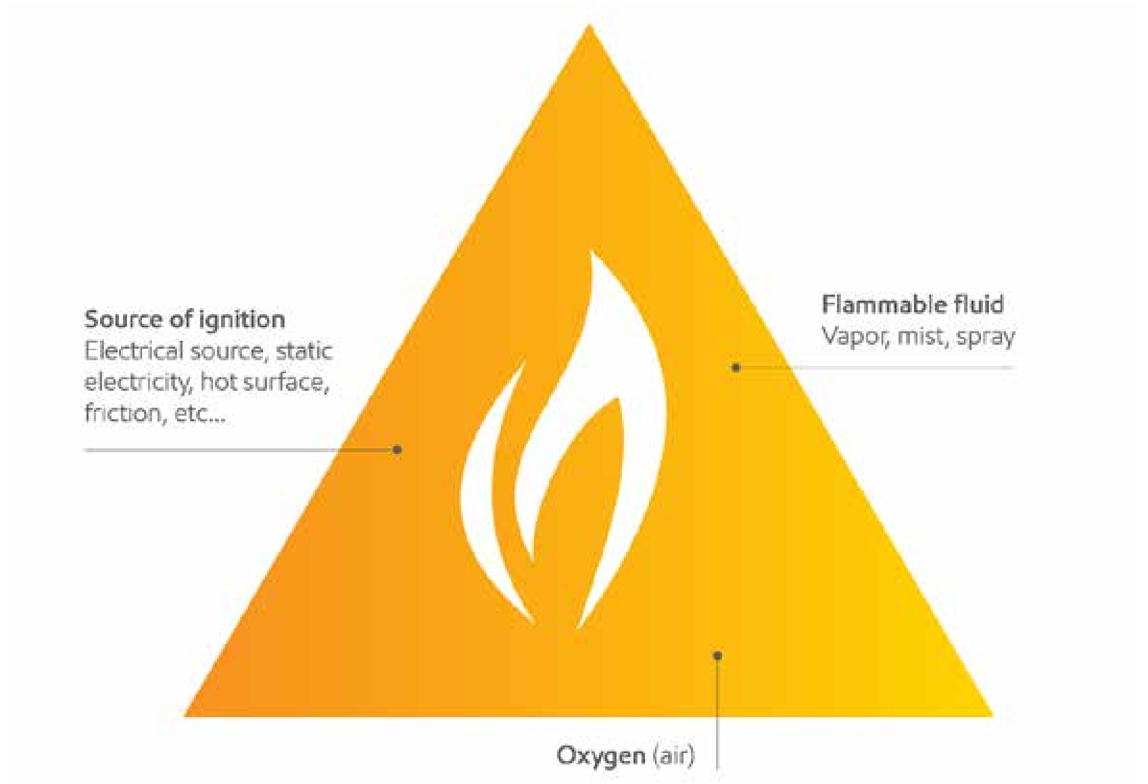
The combination of these 3 factors is necessary to generate a fire as represented by the fire triangle:



Flammable liquids

Generally, a flammable liquid can form a flammable atmosphere that can catch fire when in contact with air. Examples of flammable liquids: pentane, isopropanol (IPA), methyl ethyl ketone (MEK). Examples of nonflammable liquids: water, carbon tetrachloride.

Oxygen (air)

A flammable fluid can form a mix that is flammable only when combined with a sufficient amount of oxygen in the air. Combustion of hydrocarbons is not spontaneous and occurs only when an ignition source is present.

Source of ignition

In order to initiate the combustion reaction of flammable fluid and air, a source of energy must be present (such as a flame, a spark or even a hot surface).

A 4th element: chain reaction of combustion

For continuous combustion to occur it is necessary that the fire is fed with continuous input of fuel and oxygen in appropriate concentrations. In addition it is necessary that a continuous release of energy is provided by the reaction in order to perpetuate the chain reaction. The fire stops due to one of the following cases:

- All the fuel is depleted.
- The oxygen concentration becomes insufficient.
- The energy released is insufficient to maintain the combustion.

Physical properties and flammability limits

A number of properties are tested to measure the flammability limits of fluids.

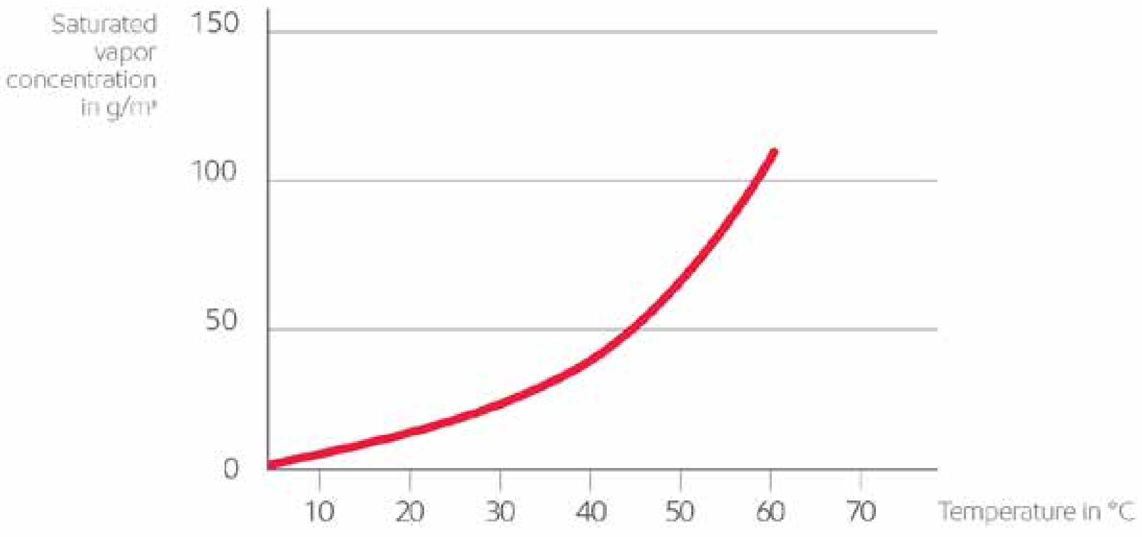
Evaporation and vapor pressure

In fact the flammable fluid molecules that burn are in the form of a vapor, not a liquid. Hence flammable liquids must evaporate in the air before they can burn: whether the mixture is flammable or not depends on the vapor concentration formed from the liquid surface. The main factor governing vapor concentration is temperature.

In a closed vessel at a given temperature, molecules will escape from the liquid to form vapor, up to an equilibrium point where the atmosphere is saturated with the flammable product vapor.

If the temperature is increased above this point, more product will evaporate: the concentration of the flammable product vapor will increase further to reach a higher saturation level.

For each liquid, a curve can be drawn of its equilibrium concentration (or saturated concentration) in the air as a function of the temperature in a closed system or vessel. This is known as the saturated vapor pressure.



Saturated vapor pressure

Evolution of the saturated concentration of Exxsol™ D40 fluid as a function of temperature

Evolution of the saturated concentration of **Exxsol™ D40** fluid as a function of temperature.

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Low Explosion Limits (LEL) and Upper Explosive Limits (UEL)

Homogeneous combustible gas-air mixtures are flammable only within a limited range of concentrations, between the LEL and UEL:

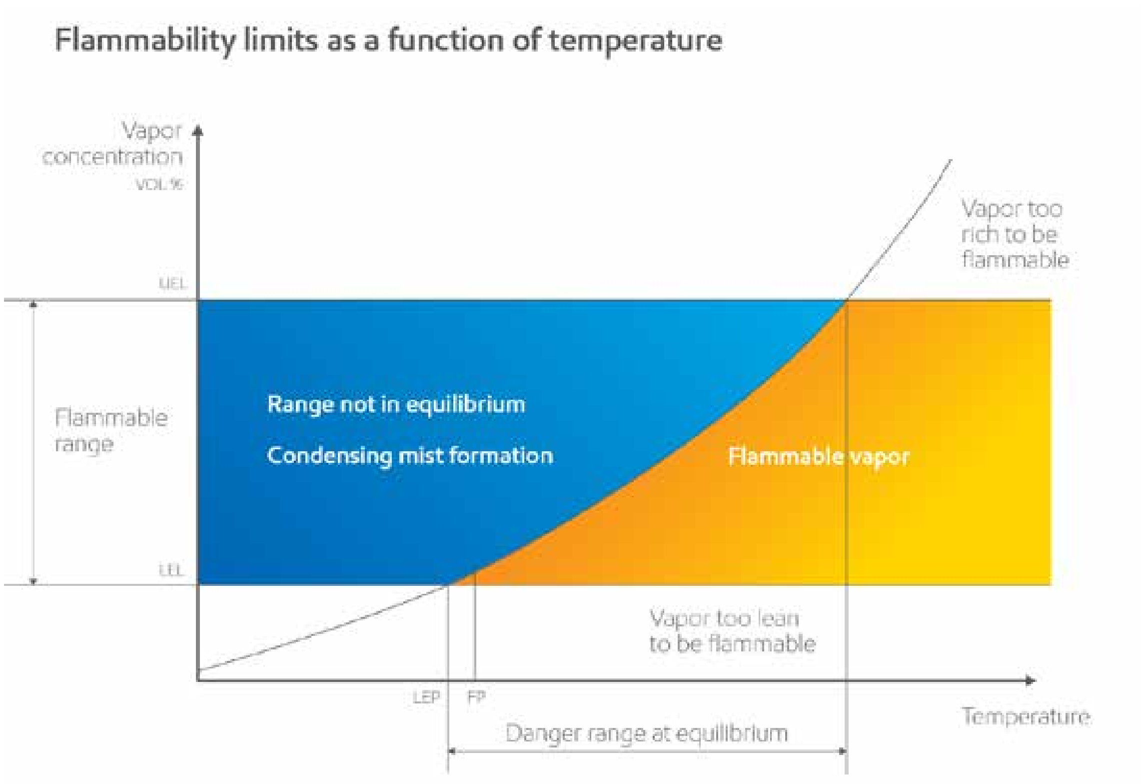
- Lower Explosive Limit: below the LEL, the quantity of flammable gas in the air is not sufficient to propagate a flame in the surroundings of the ignition source. Practically, it will not burn.
- Upper Explosive Limit: above the UEL, the concentration of flammable gas in the air is so high that there is not enough oxygen left to have the reaction of combustion propagated.
- It is in between LEL and UEL that the mixture of flammable gas and air is flammable.

These limits are presented in terms of volume percentage of flammable vapor in air.
For example, in the case of a light hydrocarbon solvent **Exxsol™ Heptane**, the flammable limits are: LEL: 1% volume; UEL: 7% volume. This means that between concentration of 1% and 7% of Heptane in air, the mixture will be flammable, i.e., it will burn throughout if exposed to an ignition source (flame, very hot surface or spark). If the concentration of heptane vapor in the air is below 1% Volume, the combustion will not occur as the mixture Heptane – air is too low to burn. If the concentration of Heptane is above 7% vol in air, the mixture is too rich to burn and combustion will not occur either.

Other examples:

- **Exxsol™ D40** has a UEL of 7.0 and a LEL of 0.6
- **Exxsol™ D110** has a UEL of 7.0 and a LEL of 0.5

The graph below summarizes the concepts, described above, of flammability limits as a function of temperature. The area comprised between the LEL and UEL concentrations and contained below the saturation vapor pressure curve are flammable. The area above the saturation vapor pressure curve is not "in equilibrium" but may exist in particular usage conditions (mist condensation, spraying, etc…) and these require specific attention.


Flammability limits as a function of temperature

Nota: Under equilibrium conditions, the temperature corresponding to the lower explosive limit is the lower explosion point (LEP). In practice, the temperature at which the vapor becomes flammable is estimated by the Flash Point test. The flash point is measured following strict standards, however not under equilibrium conditions. Therefore, the flash point temperatures is generally a few degrees above the LEP.

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Mists

In some specific cases, there is a flammability risk when operating with dispersion of fine liquid droplets in air (mists or sprays).

- In the case of **vapors**, the maximum concentration that can be reached in air is defined by the vapor pressure curve (click here) and depends on the temperature.
- In the case of a **dispersion of droplets**, the concentration of combustible material in the air is independent of the temperature, as sprays or mists are formed by mechanical actions (most often using jet pressure of a few bars or following condensation of saturated vapors resulting in droplets or mists whose particle diameter is below 0.02 mm). Click here for a visualization of the mist area (on the left side of the saturation vapor curve).

Situations where **mists or sprays** can be present **should be avoided**

Practically, situations where mists or sprays can be present should be avoided because hydrocarbon mists or sprays can be flammable at temperatures far below flash point, contrary to actual vapors which cannot ignite at a temperature below flash point. When their occurrence is likely to happen, specific safety measures have to be taken as they present a higher potential risk. It is advisable to consult specialists for the design of operations using flammable fluids.

In practice, flammability limits are not very convenient working tools as it is difficult to interpret volume concentrations in air. Generally **it is more practical to consider the flash point** of the flammable liquid and relate it to the actual temperature of use.

Vapor density

Vapor density will determine how well the vapor will be dispersed in the air after its emission. Heavy vapor will not be effectively dispersed in the air and may collect in low areas and represent a fire hazard.

Vapor density is often expressed in terms of the ratio of the gas vapor density to the vapor density of air. With air taken as unity (value=1), the vapor density ratio of the gas indicates the relative density of the vapor in the air:

Vapor density ratio =	$\frac{\text{Molecular Weight of the material}}{\text{Composite molecular weight of air (29)}}$	$\frac{MW}{29}$

Examples:

- **Exxsol™ Heptane** has a composite MW of 98. Its vapor density ratio is then of 3.4. This simple calculation indicates that Exxsol™ Heptane gaseous emissions may not homogeneously mix with surrounding air and as it is heavier than air can create high gas concentration pockets at low areas which may present a higher flammability risk.
- **Exxsol™ D40** has a vapor density of 5.0 (air=1)
- **Isopar™ H** (AM) has a vapor density of 5.3 (air=1)

Flash and fire points

In order for a flammable product to burn, its vapors have to be present in an appropriate concentration in the air, i.e., within the defined limits of LEL and UEL.

When a liquid product is exposed to air, some of it evaporates, leading to a certain vapor/air concentration. As the temperature of the liquid product is raised, more and more evaporates, and the vapor/air ratio increases. Eventually, **a temperature is reached at which the vapor/air ratio is high enough to support momentary combustion**, if a source of ignition is present. This temperature is the flash point of the product. The flash point of a fluid is therefore **the lowest temperature at which it can vaporize to form an ignitable mixture in air.**

Flash point values

For volatile hydrocarbon and oxygenated fluids, the flash point is an indication of the fire and explosion hazards associated with its use. If possible, selecting a product whose flash point is above the highest expected operational ambient temperature will ensure that no special safety precautions are necessary.

However, some light solvents have flash points below room temperature. When they are used, controlled ventilation and other specific measures are necessary to prevent the possibility of explosion or fire.

Examples:

- **Exxsol™ D40** has a flash point of 39°C
- **Isopar™ H** (AM) has a flash point of 54°C

Flash point vs. fire point

The flash point is the minimum temperature at which sufficient liquid is vaporized to create a mixture of fuel and air that will burn if ignited. As the name of the test implies, combustion at this temperature lasts only an instant – a flash. In practice, the temperature at which a flash point occurs is very close to the temperature corresponding to the LEL as shown here.

The fire point is usually a higher temperature. It is the minimum temperature at which vapor is generated at a rate sufficient to sustain combustion. In either case, combustion is possible only when the ratio of fuel vapor to air lies between the LEL and UEL limits. A mixture that is too lean or too rich will not burn even if above the minimum temperature for either point.

In most cases and for practical purposes, knowing the flash point is sufficient to determine the flammability risks associated with hydrocarbons: if the fluid temperature is above the flash point, a flammable atmosphere will be formed above its surface, providing a potential risk of explosion or fire.

> Knowing the flash point is often sufficient to determine the flammability risks associated with hydrocarbons.

Flash point measurement test methods

For most hydrocarbon and oxygenated fluids, the flash point is usually determined by a "closed cup" method, in which the product is heated in a covered container. This most closely approximates the conditions under which the products are handled in actual service. Products with flash points below room temperature must, of course, be cooled before the test is begun.

Two closed-cup methods of determining flash point are widely used. They differ primarily in details of the equipment and in the specific fields of application. However, the tests are basically similar, and may be grouped together for the purpose of description.

They are:

- **ASTM D 56** Flash Point by Means of the Tag Closed Tester
- **ASTM D 93** Flash Point by Means of the Pensky-Martens Closed Tester

The former is used for liquids with low flash points (<50°C) whilst the latter is applicable for liquids with a higher viscosity. The tests differ in the details of the equipment, the rate of heating and whether or not the test fluid is stirred.

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Auto ignition temperature

All petroleum products will burn and, under certain conditions, their vapors will ignite with explosive force. For this to happen, however, the ratio of product vapor to air must be within the defined limits of LEL and UEL.

When exposed to air, a certain amount of the liquid product evaporates, establishing a certain vapor-to-air ratio. As the temperature of the liquid increases, so do the evaporation, and thus the vapor/air ratio. Eventually, a temperature is reached at which the vapor/air ratio will support combustion if an ignition source, such as spark or flame, is present. This temperature is the **flash point** of the product.

If no ignition source is present, as the temperature increases above the product's flash point, a temperature is reached at which the product will ignite spontaneously, without any external source of ignition. This temperature is the AIT of that fluid.

Examples:

- **Exxsol™ D40** has an Auto Ignition Temperature of 259° C
- **Isopar™ C** has an Auto Ignition Temperature of 443° C

Care should be taken not to confuse flash point, fire point and AIT.

Significance of auto ignition values

The auto ignition temperature (AIT) may be used as a measure of the relative desirability of using one product over another in a high-temperature application. It is necessary to use a petroleum product with an AIT sufficiently above the temperature of the intended application to ensure that spontaneous ignition will not occur. The AIT of a product is a function of both the characteristics of the product and conditions of its environment. For example, the AIT of a substance is a function of such things as the pressure, fuel-to-air ratio, time allowed for the ignition to occur, and movement of the vapor-air mixture relative to the hot surface of the system container. In large vessels, in the case of specific wall construction materials and in close containers, ignition may occur at temperatures below the AIT determined in accordance with the standard. Consequently, the measured AIT may vary considerably depending on the test conditions.

Auto ignition temperature measurement test method

The test method generally used for measuring the AIT is the ASTM E 659: "Standard Test Method for Auto Ignition Temperature of liquid chemicals".

Ignitability and minimum ignition energy (MIE)

The ignitability of a flammable atmosphere is related to the minimum ignition energy (MIE). **MIE is the minimum amount of energy required to ignite a combustible vapor, gas or dust cloud**, for example due to an electrostatic discharge. MIE is measured in joules (J). For most materials, the lowest ignition energy value occurs at a concentration **near the midpoint between those for the lower explosive limit (LEL) and the upper explosive limit (UEL)**.

MIE serves two purposes:

- It ranks materials quantitatively in terms of their sensitivity to ignition. Materials that are readily ignited (sensitive) have a low MIE and those that are difficult to ignite have a high MIE.
- It can be compared with the available energy created by an electrical discharge that might cause an ignition.

It is prudent to assume that ignition is possible when the available discharge energy exceeds the MIE. The actual energy required for ignition may, however, be well above the MIE if the concentration of flammable material of the electrical discharge characteristics differ from the ideal.

Very low energy levels are sufficient to ignite solvent vapor/unit mixtures: as an indication, energy between 0.1 and 1 milli Joule (mJ) is generally enough to ignite vapors of hydrocarbon solvents.

Between the upper and the lower explosion limits, the ignition energy depends on the fuel concentration. Specifically the MIE is reached at conditions around the stoichiometric fuel concentration. MIE tends to decrease with increasing temperature. Most sources of ignition encountered in industrial activities will exceed the MIE of 1 mJ and require strict control.

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Static electricity

Among the sources of ignition which present a significant risk is static electricity. Static electricity builds up during the transfer of liquids especially hydrocarbon fluids. Hydrocarbon fluids are characterized by their very low electrical conductivity or correspondingly high resistivity.

As a consequence the electrical charges generated due to the motion of the fluid (for example by pumping, filtering, agitation or spraying) which accumulate in the bulk of the liquid can be quite high. In the case of low conductivity liquids, especially below 50 picoSiemens/meter (pS/m) the accumulated charges are slow to dissipate and create significant differences of electrical potential, susceptible to cause electric discharges of energy levels which are sufficient to ignite flammable vapors.

Electrical conductivity of hydrocarbon and oxygenated fluids
Hydrocarbon solvents generally exhibit electrical conductivities of below 10 pS/m which will cause a slow dissipation of the charges, requiring up to a few minutes even when proper earthing connections have been used.

Oxygenated solvents, being more polar materials, readily conduct electricity:
isopropanol (IPA) has a conductivity of about 2.106 pS/m; **methyl ethyl ketone** (MEK) has a conductivity of about 5.106pS/m.

Mitigation of static electricity risks
The risks of static electricity associated with solvents and fuels have been the subject of much academic and industrial attention, with details on prevention steps to mitigate the risks, especially:

- Earthing
- Bonding
- No-splash filling (truck tanks, drums)
- Waiting to allow dissipation of charges
- Pipe velocity limitation
- Spraying practice to take static electricity risks into account

ESIG resources, click here.

Given the complexity of the subject it is advisable to consult static electricity specialists for the design of operations using volatile flammable fluids.

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Guidelines for safe operations

Three elements are necessary for a combustion to occur, i.e., flammable source, oxygen and source of ignition. The absence of one of these three ingredients is sufficient to prevent combustion.
As a consequence, the safety measures to prevent fire risks are based on the following principles:

- Limit the concentration of flammable source in air
- Reduce oxygen content
- Eliminate ignition sources

In any case we recommend all users of flammable fluids to seek advice from a specialist to assess their situations and recommend the adequate prevention measures and emergency plans.

Limit the concentration of flammable fluid in air »

Below the Lower Explosive Limit (LEL) there are not enough vapors in the air to reach the flammability limit.

Reduce oxygen content »

For hydrocarbons, the oxygen content of the atmosphere must be reduced below 10% to make the atmosphere non-flammable.

Eliminate ignition source »

Ignition sources can be of various origins. While elimination of direct flames is often possible, preventing electrical sparks is more difficult.

Safe handling of Exxsol™ Pentane »

Pentane is highly flammable. Handling it requires knowledge of the risks involved, hardware to prevent incidents and awareness from drivers and operators.

Safe use and handling of hoses and flexible connections in the solvents industry »

Guidance Note on the specific risks when using connection hoses to transfer solvents, published by the Solvents Industry Association in the UK.

Limit the concentration of flammable fluid in air

Below the lower explosive limit (LEL) there are not enough vapors in the air to reach the flammability limit.

Operating in this range can be achieved in two ways:

- **Keep temperature below the flash point** is the easiest way and corresponds to normal practice. It is recommended to maintain a safety margin of 15°C below the flash point of the fluid.

Examples:

  - **Isopar™ G**, with a Flash Point of 42°C, can be used safely at a temperature up to 27°C (= 42-15°C). Such a 15°C margin should cover for unexpected variations such as inaccuracy of temperature control or inhomogeneities in the temperature of the liquid.
  - **Exxsol™ D100** with a Flash Point of 102°C (=102-15°C) can be used, in specifically designed equipment, at a temperature of up to 87°C without the risk of fire. Nevertheless, such equipment and operation must be critically inspected in order to ensure that several protection levels are present to correct any malfunction capable of creating a fire risk.

- **Adequate ventilation** will decrease the concentration of combustible vapors by dilution with air down to a safe level. When the temperature of use of the fluid cannot be kept at 15°C below flash point, sufficient air must be supplied by ventilation to ensure that the combustible concentration is well below the LEL (25% of the LEL is recommended).

Basics of flammability »

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Limit the concentration of flammable fluid in air

Reduce oxygen content

Eliminate ignition source

Safe handling of Exxsol™ Pentane

Safe use and handling of hoses and flexible connections in the solvents industry

Reduce oxygen content

Where flammable atmospheres can be generated and when the absence of an ignition source cannot be fully established, an inert gas (nitrogen or carbon dioxide) should be added to the vapor phase to render the atmosphere non-flammable.

For hydrocarbons, the oxygen content of the atmosphere must be **reduced below 10%**. A safety margin is further required to allow for possible variation and, in practice, the atmosphere of inert equipment must contain significantly lower levels of oxygen to fulfill safety requirements.

It is strongly recommended to check local regulations.

For **hydrocarbons**, the oxygen content of the atmosphere must be **reduced below 10%**.

Basics of flammability »

Guidelines for safe operations »

Limit the concentration of flammable fluid in air

Reduce oxygen content

Eliminate ignition source

Safe handling of Exxsol™ Pentane

Safe use and handling of hoses and flexible connections in the solvents industry

Eliminate ignition source

Ignition sources can be of various origin: any source of energy (electrical, mechanical, radiation, chemical) can ultimately be degraded into heat. While elimination of direct flames is often possible, preventing electrical sparks is more difficult:

- Flame-proof equipment should be used in any flammable atmosphere and its vicinity
- The risk of static electricity discharges must be eliminated by using proper safety devices aiming at minimizing static generation and maximizing dissipation of electrical charges. It is advisable to consult static electricity specialists for the design of operations using volatile flammable fluids.
- Heating systems must follow specific rules such as maximum flux of heat or safety devices.

While **elimination of direct flames** is often possible, **preventing electrical sparks** is more difficult.

Basics of flammability »

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Limit the concentration of flammable fluid in air

Reduce oxygen content

Eliminate ignition source

Safe handling of Exxsol™ Pentane

Safe use and handling of hoses and flexible connections in the solvents industry

Safe handling of Exxsol™ Pentane

Pentane is highly flammable. Handling it requires knowledge of the risks involved, hardware to prevent incidents and awareness from drivers and operators.

This is a summary of essential information, and the do's and don'ts you need to know to handle Exxsol™ Pentane, Exxsol™ Isopentane and blends of the two in a safe manner.

NOTE: This is only a summary of handling procedures and safety data for use of this product. Please refer to the Safety Data Sheets for complete instructions.

Summarized flammability properties

	Exxsol™ Isopentane S	Exxsol™ Pentane 80	Exxsol™ Pentane 100S
Boiling point / range	27 - 28 °C	34 - 35 °C	36 - 37 °C
Flash point	< 0 °C	< 0 °C	< 0 °C
Auto Ignition Temperature	> 250 °C	> 250 °C	> 250 °C
LEL	1.4 V%	1.3 V%	1.3 V%
UEL	7.6 V%	7.6 V%	7.8 V%

Notes: Typical values indicated in this chart describe typical physical properties and do not constitute specification limits. Test method names are available on Product Data Sheets. The typical values may vary over time.

Check it in the SDS, section 5.4

Boiling point:
According to CLP-GHS, a product having a flash point < 23°C and a boiling point ≤ 35°C is classified flammable category 1, the most stringent category.

Flash point:
The flash point of a fluid is the lowest temperature at which the fluid can vaporize to form a mixture in air that can get ignited when in contact with a source of ignition. See more

AIT:
The auto ignition temperature (AIT) of a fluid is the temperature at which the fluid will ignite spontaneously, without any external source of ignition. This temperature is above the fluid's flash point. See more

LEL / UEL:
The lowest explosive limit (LEL) and upper explosive limit (UEL) are the concentration limits between which the mixture of flammable gas and air is flammable. These limits are expressed in volume percentage of flammable vapor in air. See more

To avoid a leak or a spill, remember!

!

- Pentane will directly form a vapor cloud that can easily start a fire.
- The vapors are heavier than air and will flow to the lowest point.

✓

- Prevent any leak or spill.
- Use ventilation to prevent the formation of a flammable vapor cloud.

Basics of flammability »

Guidelines for safe operations »

Limit the concentration of flammable fluid in air

Reduce oxygen content

Eliminate ignition source

Safe handling of Exxsol™ Pentane

Safe use and handling of hoses and flexible connections in the solvents industry

Classification and labeling in the EU

Hazard identification: classification and labeling in the EU

	Hazard categories	Label pictogram Signal word	Hazard statements
Exxso™ Isopentane S	Flam. Liquid 1, Aquatic Chronic 2, Aspiration Tox. 1, STOT SE 3 (narcosis)	 Dgr	H224, H411, H304, H336, EUH066
Exxsol™ Pentane 80	Flam. Liquid 1, Aquatic Chronic 2, Aspiration Tox. 1, STOT SE 3 (narcosis)	 Dgr	H224, H411, H304, H336, EUH066
Exxso™ Pentane 100S	Flam. Liquid 1, Aquatic Chronic 2, Aspiration Tox. 1, STOT SE 3 (narcosis)	 Dgr	H224, H411, H304, H336, EUH066

Dgr stands for Dangerous goods regulations

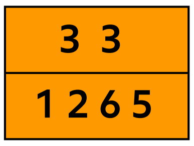
Check it in the SDS, section 2

Transport classification

	UN Number	Packaging group	Class/Div. or Label(s)	EHS / Marine Pollutant (Yes/No)	Classif. code
Exxso™ Isopentane S	1265	I	3	Yes	F1
Exxsol™ Pentane 80	12654	I	3	Yes	F1
Exxso™ Pentane 100S	12654	I	3	Yes	F1

Dgr stands for Dangerous goods regulations

ADR / RID / IMDG Class 3, Packaging group I, UN number 1265



International Carriage of Dangerous Goods by Road (ADR)
International Railway Transport of Dangerous Goods (RID)
International Maritime Transport of Dangerous Goods (IMDG)

Check it in the SDS, section 14

Basics of flammability »

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Limit the concentration of flammable fluid in air

Reduce oxygen content

Eliminate ignition source

Safe handling of Exxsol™ Pentane

Safe use and handling of hoses and flexible connections in the solvents industry

Safe handling and storage

Throughout the entire transport process – from the vehicle specifications to the loading/unloading, down to the reporting – safety and security must be the top priority.

Personal protective equipment (PPE)	
Drivers	Drivers should always wear appropriate PPE at the loading AND unloading sites: **Standard PPE:** ▪ Approved safety helmet; ▪ Safety shoes : EN 20345 S3, closed (high-laced recommended); ▪ Coverall – flame retardant, chemical resistant, anti-static, fully covers the arms and legs; ▪ Safety glasses with side shies. Additional PPE in case of direct exposure to the product: ▪ Chemical resistant gloves, e.g., Nitrile. See more
	Refer to Cefic guidelines
	Check it in the SDS, section 8.2

Before loading	
Vehicle	**Regulations requirements:** • Meet the ADR requirements for class 3 products; • For bulk liquid containers (BLC): be U.N. portable tanks with 4 bar working pressure and 6 bar test pressure. **Equipment:** • Steel tanks and chassis versus aluminum for higher road accident resistance; • Vapor return connections; • Conductive hoses in an enclosed hose rack; • A proof of pressure testing to the legal requirements shall be available on the vehicle; • Vacuum vent.
Drivers	• Must be ADR certified; • Must have the appropriate PPE available.

Loading at the plant	
Vehicle	• Must be earthed (grounded); • Vehicle electricity must be switched off.
Drivers	Personal protective equipment (see above): **Vehicle control:** • Check that bottom valves and butterfly valves are closed and end caps are tight (top loading); • Prior to this, gaskets will have been checked.
Facilities	• All ignition sources must be avoided and are forbidden (smoking, open fire, mobile phones, etc.). All permanent facilities must be earthed (grounded); • A site operator must be available at the loading area during the full loading operation and must check if equipment is ready for transport.
	Refer to Cefic guidelines

After loading	
Drivers	• Check if the vehicle has the correct placards; • Label the vehicle accordingly if it is using a nitrogen blanket; • Check for leaks.

During transport	
Drivers	• Comply with legal requirements (speed limit, resting time, no alcohol and drugs, no mobile phone during driving, etc.); • Behave according to defensive driving principles e.g., European Chemical Industry Council (Cefic) behavior-based safety guidelines; • Make sure drivers can identify themselves with photo ID; • Do not pick up hitchhikers or stop for suspicious persons; • Keep in touch with logistics planners/dispatchers; • Never leave the vehicle unattended; always stop in guarded parking at night; • Check if the valves and end cap are in the correct position and tight; • It is advisable that the driver stays with the vehicle whenever possible, even on a sea ferry.

Basics of flammability »

Guidelines for safe operations »

Limit the concentration of flammable fluid in air

Reduce oxygen content

Eliminate ignition source

Safe handling of Exxsol™ Pentane

Safe use and handling of hoses and flexible connections in the solvents industry

Unloading at customer	
	- Don't hesitate to stop -- or not even start -- the operation if one of the requirements below is not satisfactory, or could lead to an unsafe situation
Drivers	- Before unloading, introduce the driver to all safety and emergency procedures; - Position the vehicle so that the driver can easily drive forward in an emergency; - Drivers must wear helmets, safety shoes, safety glasses, coveralls and gloves; - The driver must attend the full unloading operation and not stay in the cabin.

Unloading technique	- Unload only by pumping, pushing with nitrogen or by gravity;
	- For underground tanks, unloading by gravity is simpler and safer;
	- When unloading by pump, use customer's pump to avoid a running truck ignition source;
	- Unloading by air compressor is strictly prohibited!;
	- Unloading by nitrogen is not preferred:
	  - It doesn't allow the use of a vapor balance line;
	  - It adds risks during and after unloading;
	  - The vehicle should be labeled with the appropriate N2 danger signs afterwards;
	- All permanent facilities must be earthed (grounded).

Vehicle	- Trucks must be earthed; It is recommended to have an indicator to confirm adequate earthing (grounding) with auto shut-off of discharge operations; - Truck electricity must be switched off; - A vapor return system must be used, after connection of the hoses, first open vapor line before the product line; - Hose connection to the truck must be done by the driver; - Opening the manhole is strongly discouraged as the slightest static electricity can ignite vapors; - If it is absolutely necessary to open the manhole, use a portable LEL detector; a flammable gas detector is always recommended; - All ignition sources must be avoided.
Customer responsibility	- A site operator must be available at the unloading spot during the full loading; - Unloading is to be done at least 25m from buildings and other activities; - Fire-fighting equipment and absorbent material must be available at the unloading spot; - Wear the appropriate personal protective equipment (see above); - Fence off the area; - Stop all other activities around the unloading spot (hot work, etc.); - Check that the correct product is delivered into the correct tank; - If sample taking is really unavoidable, it must be done via the customer installation by qualified site personnel; - Samples must be taken from a sample point in the fixed piping by qualified personnel; - Check the quantity and tank level, be sure the quantity will fit in the tank; - Connect the truck to the customer installation; - Only conductive hoses must be used; - Check equipment status before unloading (earthing, hoses, etc.); - Attend the entire unloading operation.
	Refer to Cefic guidelines

Basics of flammability »

Guidelines for safe operations »

Limit the concentration of flammable fluid in air

Reduce oxygen content

Eliminate ignition source

Safe handling of Exxsol™ Pentane

Safe use and handling of hoses and flexible connections in the solvents industry

After unloading	

	• An empty and unclean truck or BLC remains subject to transport of dangerous goods;
	• Vehicles and drivers must be ADR certified;
	• Return document must be signed off;
	• Document must be accompanied by:
	  • Declaration for transport of dangerous goods;
	  • ExxonMobil Chemical emergency response telephone list;
	  • Safety Data Sheet.

Processing and storage	
Customer responsibility	• **ExxonMobil assesses customers readiness to handle pentane through a detailed questionnaire** Prior to supplying ExxsolTM pentane products to customers, ExxonMobil systematically assesses, through a very detailed questionnaire, their ability to deal with all associated risks. The questionnaire covers topics such as storage permits, fire fighting facilities, truck equipment, unloading facilities, operations and processes in place, etc. • **The processing and storage of dangerous goods falls under the Seveso III Directive in Europe** ExxsolTM pentanes are captured by Seveso III if the quantity of product stored on any individual site exceeds set thresholds.

What to do in case of a fire or a spill

In case of a fire or a spill, it is critical to apply the following emergency measures:

In case of a fire	• Engage fire alarm; • Shut down all operations; • Protect people, evacuate to a safe location; • Fence off the area and prohibit entry; • **Use dry powder, foam or carbon dioxide (CO2) to extinguish flames;** • **Only use water spray to protect people, to cool down surfaces exposed to the fire/heat or to disperse vapors;** • Do not apply straight streams of water on a product pool! Check it in the SDS, section 5

Basics of flammability »

Guidelines for safe operations »

Limit the concentration of flammable fluid in air

Reduce oxygen content

Eliminate ignition source

Safe handling of Exxsol™ Pentane

Safe use and handling of hoses and flexible connections in the solvents industry

In case of a spill	- Engage fire alarm; - Shut down all operations; - Prevent ignition sources; - Fence off the area and prohibit entry; - Prepare for a fire; - Stop the leak (shutdown pumps, close valves, etc.); - Contain the spilled product (close sewers, use booms and absorption material); - Recover the product with appropriate absorbents; - **Only use water spray to disperse the vapors and to protect personnel attempting to stop a leak;** - Do not use water on the spilled product! Check it in the SDS, section 6

Report incidents and near misses

To help drive the highest level of safety and security, it is important that **you report all incidents and near misses** around security, safety, health and environment (SSHE) during loading, transport and unloading. Near misses and safety observations must be reported via your company system; these are as important as incidents since they can avoid an accident from occurring in the future.

Serious incidents, which need support from ExxonMobil, must be reported to the ExxonMobil emergency response number of the country where the incident has happened; contact details are mentioned on the SDS

Using this information and more, ExxonMobil will provide advice to the transporter and relevant authorities on the risks of its transported product.

Check it in the SDS, section 6.1

For further details on Exxsol™ pentanes please download their Safety data sheets (SDS)**:**

- Exxsol™ Isopentane S SDS
- Exxsol™ Pentane 80 SDS
- Exxsol™ Pentane 100S SDS

Safe use and handling of hoses and flexible connections in the solvents industry

View PDF here

Human health

We see it as our responsibility to understand the potential risk to humans if they are exposed to chemical substances. Our industry complies with risk management processes that are as strict as those used in the medical and pharmaceutical industries to ensure that product safety standards are maintained at their highest level. This section explains the main toxicology concepts and tests underlying such processes.

Basics of human toxicology »

Human exposure assessment »

VOCs indoor air quality »

Basics of Human Toxicology

The physician Paracelsus (1493-1541) was the first to say that “Dosis sola facit venenum,” usually translated as: “All substances are poisons; there is none which is not a poison. The right dose differentiates a poison and a remedy.” Human toxicology evaluates potential effects of natural or synthetic substances on human health. They can be found in numerous locations such as the foods we eat, the air we breathe, the products we use at home and at work and many more. Today, toxicology has very practical applications. Many industrial toxicology studies are conducted to satisfy regulatory requirements and to provide data for setting the conditions and limits for the safe handling, use and disposal of substances. Our focus in this resource guide is on synthetic chemical substances.

Key concepts of toxicology »

Concepts such as dose and exposure, metabolic capabilities, substance threshold and human relevance are considered when assessing the toxicity of substances.

Testing for human relevance »

An essential question facing toxicologists and risk assessors is: how relevant are results from high-dose laboratory studies for predicting potential human health effects?

Expression of Results »

Different expressions of results are used: LD50 or LC50 for acute toxicity studies and NO(A)EL for sub-chronic studies and others.

Animal Welfare »

We take animal welfare very seriously and limit animal testing by using alternatives (in vitro tests) as much as possible, and continually assessing other substitute tests.

Testing Guidelines and GLP »

Detailed guidelines describing the design and conduct of toxicological studies are available. Studies should follow the principles of Good Laboratory Practice (GLP).

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Key concepts of toxicology

A few concepts that underpin toxicology are absolutely critical to determine the hazards of substances and the risks that may be associated with their use. Each of these concepts should be taken into consideration when testing for substance toxicity.

Dose and exposure

Chemicals may enter the body in different doses and in various ways, or routes of exposure.

Routes of exposure are important because they can alter a chemical's hazard profile and include:

- **Inhalation**: absorption of vapors primarily through the respiratory tract if inhaled
- **Skin contact or eye contact**: absorption or injection through the skin or eyes, primarily via contact with liquids
- **Ingestion**: absorption through the digestive tract, which can occur for example through eating or smoking with contaminated hands or in contaminated work areas.

A **safe dose** is a dose level at or below which **no adverse effect is expected**.

Every material can also cause harm (i.e., is toxic) at some dose level. The following examples show how levels at which chemicals are toxic can differ greatly:

Examples:

- **Sodium chloride** (table salt) is lethal to rats if given at very high doses. The dose which would kill half of the treated rats (expressed as the lethal dose-50 or LD50) is 4,000 milligrams/kilogram body weight/day. This corresponds to a teaspoonful of salt per day.
- **Nicotine** (a chemical found in tobacco) is much more toxic to rats than sodium chloride. The LD50 for nicotine is 50 milligrams/kilogram/day, making it approximately 80 times as toxic to rats as is sodium chloride. This is the equivalent of a tiny pinch of nicotine per day.

Note that doses are usually expressed as a quantity per day and relative to the animal body weight to enable comparison of effects across species of different sizes.

A "safe dose" is a dose level at or below which no adverse effect is expected. It is called a "substance threshold", usually expressed as a NO(A)EL.

Metabolic capabilities

The ability of an organism to metabolize (biochemically convert) and change a chemical can have a significant effect on the potential of a substance to cause harm – in different ways:

- Chemicals can sometimes be metabolized to forms which are either more or less toxic than the chemical itself. This shows how metabolic processes can either create or remove toxic substances.
- Metabolism can also influence the time it takes for a chemical to be removed from the body. In general, the quicker a substance is eliminated, the less likely it is to cause a toxic response.

Examples:

- **Polycyclic aromatic hydrocarbons** (PAHs) such as benzo-(a)-pyrene, while not carcinogens themselves, are metabolized in mammals to carcinogenic substances.
- **n-Hexane** can be metabolized to form 2,5-hexanedione, which is the ultimate neurotoxic form of the molecule.

Substance threshold

For every chemical substance there is a threshold (or finite level) at or below which no adverse effects would be expected. In essence this is the definition of a safe dose.

Example:
Perchloroethylene (a dry-cleaning solvent) causes liver damage in mice when administered orally at dose levels at or above 100 mg/kg/day for several weeks. However, no liver damage is detected in mice exposed to lower doses.

> A **threshold** or **safe dose** is one at or below which **no adverse effects** would be expected.

A basis for defining Occupational Exposure Limits (OELs)
The threshold is also commonly called the **NO(A)EL** or **NO(A)EC**, the No Observed (Adverse) Effects Level or Concentration. It is the highest substance level or concentration at which no adverse effects are detected. It is how study results are expressed, especially in sub-chronic studies, and also often used as the basis for setting Occupational Exposure Limits (OELs). In certain cases, the Lowest Observed (Adverse) Effect Level **(LO(A)EL)** or Lowest Observed (Adverse) Effect Concentration **LO(A)EC** can be used. It is the lowest level at which effects are observed.

No threshold for mutagenic and certain carcinogenic agents?
The threshold concept may not apply to mutagenic and certain carcinogenic agents such as ionizing radiation and benzo-(a)-pyrene. These agents interact with genetic material, or DNA (deoxyribonucleic acid), causing sometimes permanent damage and a mutation. Mutations can result in the conversion of normal cells into pre-cancerous ones. In theory, one molecule of a mutagenic chemical could cause a mutation in a gene that could ultimately result in cancer. There are many steps from DNA damage to tumor development, including metabolism and DNA repair, which have their own thresholds.

In practice, even for mutagens and carcinogens acting via gene mutation, a practical threshold exists. An example is radiation where prolonged exposure over many years to nuclear reactors or use of radio-isotopes for medical purposes can cause gene mutation. Yet, practical thresholds are applied in the workplace to prevent risks of developing cancer. Similarly, drugs used in chemotherapy to treat cancer kill cancer cells, but some can also be mutagenic and cause cancer. So while in theory there is no threshold for mutagens, genotoxic carcinogens and radiation, there is a practical threshold.

Because scientists do not know yet whether this carcinogenic process has a threshold or not, it is assumed that there are no absolutely safe doses for carcinogens that act via mutational processes.

Human relevance and other factors

Most of the information on toxicology comes from studies with laboratory animals or other alternative systems. However, laboratory animals are not humans and laboratory experimentation is not the real world. It is therefore critical to think about whether the laboratory data are truly indicative of hazard and consider the **importance of mechanisms**, i.e., the ways in which a substance causes an effect.

Examples:

- Some of the effects observed in laboratory animals can never occur in humans due to genetic, metabolic or physiologic differences between humans and animals.
- Sometimes effects observed in animals could in principle also occur in humans exposed under similar circumstances, but the conditions of the laboratory studies can be so extreme that similar exposures in humans are unlikely, if not impossible.

> When **assessing hazard**, it is critical
> to consider the **importance of mechanisms**.

In some cases – depending on the substance tested, the severity of the effects and the experimental conditions – further tests and investigations are required to assess human relevance.

Other factors affecting response to chemicals

Besides the concepts of dose, exposure, metabolic capabilities or substance threshold, other factors can affect how a body responds to chemicals:

- Differences within species. For example, some individuals in the human population are allergic to penicillin while others are not.
- The speed at which a toxic dose is delivered and/or the route of exposure.
- A person’s age can affect the capacity to repair tissue damage.
- Previous exposures can lead to changed tolerance or sensitivity.
- General state of health, physical condition and life style.

Testing for human relevance

One of the major questions facing toxicologists and risk assessors is: how relevant are results from high dose laboratory animal studies for predicting potential human health effects?

The answer lies in various studies:

- Study of pharmacokinetics, that is the absorption, metabolism, and elimination of chemicals.
- Study of the mechanisms by which chemicals produce specific toxic effects in humans, tissues and cells from humans and animals.

It should be noted that non-animal testing is preferred, whenever possible. Animal testing is undertaken only as a last resort and where necessary to ensure safe use of a product.

Pharmacokinetics

Pharmacokinetics is the study of the movement of materials into, through and out of organisms. Pharmacokinetic studies examine the uptake (absorption), distribution (localization to target organs), metabolism (breakdown) and excretion of chemicals.

Knowledge of pharmacokinetics enables toxicologists to better use the information from animal studies to predict the potential for effects in humans. Understanding metabolism is important because it is the way organisms convert chemicals to either more or less toxic metabolites.

For many substances, toxicity occurs only at high doses which overwhelm or saturate the detoxification metabolic pathways. Saturation of detoxification pathways may occur at the high dose levels used in the rodent cancer bioassays and other animal studies.

Therefore, when extrapolating the results of animal tests to humans and high dose levels to low doses, it is important to consider differences in pharmacokinetics.

Expression of Results

Depending on the test performed, many different expressions of results are used. Here is a selection of the most frequently used expressions.

Acute toxicity studies:
Acute toxicity test results are usually expressed as the LD50 or LC50 , i.e., the Lethal Dose (LD) or Lethal Concentration (LC) that results in mortality in 50% of a group of laboratory animals:

- The **LD50** is normally expressed as the amount of test substance administered per kilogram (kg) of body weight, thus allowing effects in animals of different sizes to be compared.
- The **LC50** value is expressed as the concentration of the test material in the air (ppm or mg/L) over a specific treatment period (normally 4 hours).

Other studies, in particular sub-chronic toxicity studies:
In other animal studies, in particular sub-chronic toxicity studies, it is common practice to express the results in terms of:

- The **NOEL (or NOEC)** is the no-observed-effect level (or concentration) and the highest level at which a substance can be given without producing any effect at all. It is sometimes necessary to distinguish it from the NOAEL (or NOAEC).
- The **NOAEL (or NOAEC)** is the no-observed-adverse-effect level (or concentration). It indicates the highest dose level or concentration of an agent that can be given without producing toxic or adverse responses.
- The **LOEL (or LOEC)** is the lowest-observed-effect level (or concentration), the lowest dose level at which an effect is observed.
- The **LOAEL (or LOAEC)** is the lowest-observed-adverse-effect level (or concentration) or the lowest dose level of the test material that caused evidence of an adverse effect.

Different tests are potentially associated with **different expression of results**.

Adverse and non-adverse effects

- **Adverse effects** are the ones related to changes in structure or function of specific organs which are likely to lead to organ damage or functional impairment. They may be due to repeated effects of chemical exposure or to the buildup ("accumulation") of toxic metabolites of the chemical in one or more target organs. It may require weeks to months of exposure for repeated dose effects to develop. Possible changes which may be indicative of adverse effects include: significant changes in body and/or organ weights, alterations of hematology (blood), clinical chemistry, and serum enzyme levels, observations of associated tissue pathology (histopathology).
- **Non-adverse effects** are physiological adaptations or incidental, usually related to high doses used in animal experiments. Normally these disappear once exposures stop and have no health consequence.

Example: carbon tetrachloride, a chlorinated substance once used as a solvent

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Laboratory animals were exposed to vapors of carbon tetrachloride at dose levels of 5, 10, 25, 50, 100, 200 and 400 ppm, seven hours/day, five days/week for up to six months. Treatment caused increases in liver weight and development of fatty liver at concentrations of 10 ppm and higher. The development of fatty liver which was a harmful (i.e., adverse) effect was observed at all exposure levels greater than 5 ppm. The dose level of 5 ppm had no ill effect on the rats and guinea pigs under the conditions of the study. Therefore, the **NOAEL** is 5 ppm and the **LOAEL** is 10 ppm.

No effect level

At times, some effects are the consequence of normal physiological properties and not adverse effects. There are times when results are referred to as "No Observed Effect Levels", or "NOELs" to indicate that effects were observed at the stipulated doses but that they were not necessarily harmful.

Animal Welfare

ExxonMobil Chemical believes firmly in the principle that the potential hazards of its products must be understood and that the risks must be assessed in studies of appropriate design, including, when necessary, those involving animals.

However, the company takes animal welfare very seriously and limits as much as possible tests that involve them. Instead, we use suitable alternatives or replacements (such as testing in vitro) whenever they are available and reliable. We are also actively involved in alternative test development.

When animal testing cannot be avoided, we seek opportunities to reduce the population number and amount of tests conducted and to refine the information gained from each test. For example, we share testing data to study generic examples and avoid excessive numbers of tests.

ExxonMobil Chemical follows the OECD guidelines on animal welfare

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Testing guidelines and GLP

Detailed guidelines describing the design and conduct of physicochemical, toxicological and ecotoxicological studies are available. The major guidelines are:

- Organization for Economic Cooperation and Development (OECD) Guidelines for the Testing of Chemicals
- U.S. Environmental Protection Agency (EPA) Health Effects Test Guidelines
- U.S. Food and Drug Administration (FDA) Toxicological Principles for the Safety Assessment of Direct Food Additives and Color Additives Used in Food, also known as the "Red Book"

Good Laboratory Practice (GLP)
All toxicological studies performed to satisfy regulatory requirements and support product safety should be conducted according to the principles of GLP. The GLPs describe a set of organizational processes, data documentation steps and systems required in laboratories to ensure that studies are of an acceptably high quality. The main areas of GLP regulation are:

- Test facility organization and personnel
- Quality assurance program and personnel
- Facilities
- Equipment, materials and reagents
- Test systems
- Test article and reference (control) substances
- Standard operating procedures
- Performance of the study and protocol adherence
- Reporting of study results
- Storage and retention of records and materials

The GLP regulations and guidelines now in place include:

- The OECD Principles of Good Laboratory Practice (GLP)
- In the EU:

  - Directive 2004/9/EC on the inspection and verification of good laboratory practice (GLP)
  - Directive 2004/10/EC on the harmonisation of laws, regulations and administrative provisions relating to the application of the principles of good laboratory practice and the verification of their applications for tests on chemical substances

- In the U.S.: EPA and FDA Good Laboratory Practice regulations

Human exposure assessment

Whereas laboratory studies provide the data necessary to define chemical substance-related hazards, exposure assessment evaluates the degree of risk when an organism comes in contact with a chemical. It involves generating exposure scenarios that estimate the magnitude of exposure to a substance under conditions of use. This enables the safe dose or concentration of a substance to be determined for which people or the environment may be exposed.

REACH in Europe and TSCA in the United States require that substances are evaluated on the basis of risk as well as hazard. In the framework of REACH, manufacturers and importers are legally required to carry out exposure assessments of substances that are classified as "dangerous" or of PBT or vPvB substances. Manufacturing and all identified uses of the substances must be covered.

Examples of human exposure scenarios could include:

- Workers exposed to chemical substances in a workshop.
- Consumers exposed to chemicals in household products.
- A community being exposed to chemicals from a nearby manufacturing facility.

Key concepts »

The key concepts are exposure, dose of substance to which organisms may be exposed, as well as exposure determination methods.

Assessment methodology »

The methodology used to assess exposure relies on a systematic process: planning, data gathering, quantification of exposure.

Occupational exposure assessment »

Occupational exposure assessment is concerned with the prevention and management of health and safety hazards in the workplace and the systematic management of industrial hygiene information.

Consumer exposure assessment »

Consumer exposure assessment evaluates exposures to the general population from contact with a wide range of consumer products.

Community exposure assessment »

Community exposure assessment is applicable to evaluating potential chemical risks to communities adjacent to a nearby manufacturing facility.

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Key concepts

In human exposure assessment, the key concepts are:

- Exposure and the different routes of entry into the body
- The dose or amount of substance to which organisms may be exposed
- Exposure determination methods

Routes of exposure and dose
Chemicals may enter the body in different doses and in various ways (or routes of exposure). Routes of exposure are important because they can alter a chemical's hazard profile and include:

- Inhalation: absorption of vapors primarily through the respiratory tract if inhaled
- Skin or eye contact: absorption or injection through the skin or eyes, primarily via contact with liquids
- Ingestion: absorption through the digestive tract, which can occur for example through eating or smoking with contaminated hands or in contaminated work areas.

Every material can also cause harm (i.e., is toxic) at some dose level.

Exposure determination calculation
Exposure can be expressed as the product of a substance's concentration times the duration of contact or as an average daily dose across all routes of exposure. For more detail on the calculations, see below.

Definition of different types of doses

Due to the complexity of absorption of substances by a human organism, a number of different but related **dose levels** need to be defined.

- The **applied dose** is the amount of a chemical that is available for absorption at the exposed area. Since the applied dose is often difficult to measure directly, a surrogate, called the **potential dose**, is often used.
- The **potential dose** is the amount of a chemical that would be absorbed if it were 100% bioavailable. Absorption factors are typically applied to the potential dose that estimate the amount of the chemical that has been absorbed by one or more of the routes of exposure and is available for interaction with biological receptors. This amount is the **internal dose**.
- Once absorbed, the chemical can undergo metabolism, storage, excretion, or transport within the body. The amount transported to an individual organ, tissue, or fluid is termed the delivered dose. The **delivered dose** may be only a small part of the internal dose.
- The **biologically effective dose**, or the amount that actually reaches cells, sites, or membranes and produces an effect, may only be a part of the delivered dose, but it is obviously the crucial part.
- A direct indicator of an individual's **internal dose** is determined through **biological monitoring**, or **biomonitoring**. This involves sampling and analysis of the individual's body fluids or tissues to measure the internal concentration of a substance. The internal sample of an individual's exposure to a chemical substance is often referred to as a **biomarker**.

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Exposure calculation

Exposure can be expressed in different ways:

- As the product of a substance's concentration multiplied by the duration of contact
- As an average daily dose combined across all routes of exposure

Substance's concentration x duration of contact

Since exposure concentration can vary over time the equation for exposure is represented as an integral:

$E=\int_{t_1}^{t_2} C(t)dt$	Where:		
	E	=	integrated or magnitude of exposure
	C(t)	=	exposure concentration as a function of time
	t_1, t_2	=	start and end time for the exposure
	The time difference between t1 and t2 is the exposure duration		

A typical unit for exposure might be **(mg/m3) x hr**.

Average Daily Dose

Time-weighted average exposure is often used to describe exposure in risk assessments. It is the integrated exposure divided by the period during which the exposure occurs.

As it is usually normalized for a person's body weight, the units for the time-weighted average exposure might be milligrams per kilogram per day, or **mg/kg/day**. In this form, the exposure is more accurately referred to as a dose.

An example is the Average Daily Dose, or ADD. The ADD can be related directly to toxicological metrics, such as the reference dose, for quantifying risk.

The average daily dose across all routes of exposure can be calculated from a general equation:

$ADD = \sum \frac{(C_m)(IN_m)}{bw}$	Where:		
	ADD	=	average daily dose (mg/kg/day)
	C_m	=	concentration of chemical in medium m (mg/kg or mg/m^3)
	IN_m	=	total daily intake rate for medium m (kg/day or m^3/day)
	bw	=	body weight (kg)

By summing the doses for each exposure media, the total daily dose is obtained.

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Assessment methodology

The methodology used to assess exposure relies on a systematic process:

- Planning
- Data gathering
- Development of exposure scenarios
- Determination of exposure

Planning an exposure assessment

As the objective of an exposure assessment can range from an occupational exposure assessment of workers in industry to consumer exposures to chemicals in household products, **there is no single methodology for conducting one**. However, exposure assessment, like any other scientific discipline, requires that **sound scientific principles** are applied to sampling and analysis.

When planning an exposure assessment, there are basic considerations that the assessor should address, including:

1. Purpose
2. Scope
3. Level of detail
4. Approach – direct or indirect measurement method

Exposure assessment requires that sound scientific principles are applied to sampling and analysis.

Purpose:

- Why is exposure being assessed?
- What questions will the study address and how will the results be used?

Scope:

- What are the boundaries of the exposure assessment?
- What substances will be assessed, in which media, over what time period?
- Who will be monitored?
- What routes of exposure will be assessed, by what method?

Level of detail:

- How accurately must the exposure be calculated?
- Is this to be a screening-level study, or a more refined exposure assessment?
- Are there limitations to the precision of the information that can be collected to assess the exposure?

Approach:

- Will the approach be satisfactory to address the purpose and scope of the assessment at the desired level of detail for the group of people to be assessed?
- Which approach – direct or indirect measurement method – will be appropriate.

Direct methods
Direct methods include **personal monitoring or biomonitoring**. They measure the exposure at the point of contact, or in the case of biomonitoring, after uptake has occurred through one or more points of contact.

Indirect methods
Indirect methods include **environmental monitoring** coupled with relevant peripheral data on **biological and physical characteristics**.

- Biological and physical characteristics of the **subjects**, such as body weight, breathing rate or skin surface area
- Physical characteristics of **exposure** (or **exposure factors**), relating to human activities, such as time spent at home or at work or how often a task is conducted per day

Compilations of exposure factors can be found in the following publications:

- Exposure Factors Sourcebook for European Populations (with Focus on UK data) (ECETOC 2001)
- The U.S. Environmental Protection Agency's Exposure Factors Handbook (USEPA 2011)

Data gathering

The data required to assess exposure will generally be different for a study of occupational exposures versus a study of a community beyond the fence-line of a facility.

Data collection for an exposure assessment can either be specific to the study being conducted or use data previously collected from other studies.

Sampling plan
Planning a new specific study requires the development of a sampling plan.

Ideally one would like to measure the personal exposure of every person in an investigation at every possible time period. As this is not possible, a limited number of samples or measurements, either from personal or from fixed monitors, are taken. They are then extrapolated to represent the study population.

A good sampling plan should consider the number, location, and times that samples are to be collected, the scenarios, and quality control considerations.

Although the methods for collecting data for an exposure assessment using the direct method are different than the methods for data collection for an indirect exposure study, the data parameters needed for estimating exposure, such as substance concentration during exposure or duration of contact with the substance, are the same.

Data collection can either be **specific to the study** being conducted or from **previously-collected data** from other studies.

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Substance concentration during exposure

Substance concentration is important for estimating exposure regardless of the route of exposure. Measured concentrations can either be at the point of contact, or can be concentrations measured in various environmental media (e.g., air, water, dust).

Duration of contact with the substance

Inhalation and dermal exposures usually represent the key routes of exposure for occupational studies.

- Inhalation: for estimating inhalation dose or uptake, an estimate of the inhalation rate, specified in units of volume of air breathed per time, is needed.
- Dermal contact: an estimate of the skin surface area and the rate of dermal uptake, specified by a permeability rate, are needed.
- Ingestion: for estimating ingestion, an estimate of the ingestion rate, specified in units of mass of food per time, is needed.

In order to estimate the potential dose, additional exposure factors are needed. Further information may be needed to estimate exposures depending upon the exposure scenario.

Frequency distributions

Frequency distributions of the exposure data are obtained in two ways:

- Using relevant statistical tools
- Selecting discrete values from the ranges of the exposure data to quantify exposures

The second alternative is simpler and often used for assessing occupational exposures to chemicals or other agents. In such a case, the exposure factor values chosen are high and the inclusion of this series of high exposure factors results in what is referred to as a reasonably worst case scenario. **The presumption is that if the reasonably worst case exposure scenario does not present any significant health concerns, then no further analysis is necessary**.

Development of an exposure scenario

An exposure assessment is typically based upon defined exposure scenarios (ES) that describe real-life exposure situations. Historical exposures can be recreated based upon past conditions. Future exposures can be estimated based upon potential impacts of various control actions.

The information needed to define an ES generally includes:

> An exposure assessment is based on **defined exposure scenarios** that describe real-life exposure situations.

Physical setting where the exposure takes place

It usually includes details about the time and location of the exposure. For example, if the exposure takes place indoors, factors such as the size of the room where the exposure occurs, the ventilation system, the duration of exposure, etc. are important to determine the concentration of the substance.

Exposure pathway from source(s) to exposed individuals
It is the path a chemical or physical agent takes from source to exposed organism; it typically starts with the source of a release, a transport medium, the exposure point, and the route of exposure.

Characterization of the chemical or agent
It includes any data relevant to estimating exposure. The source strength, the time variation of chemical concentrations, the locations of exposure, the exposure pathway, fate of the chemical, and any other information deemed relevant.

Identification of the individuals or population exposed
Individuals and the profile of contact with the chemical or agent are based upon behavior, location as a function of time, and characteristics of the individuals themselves.

Estimation of dose
The dose is to be calculated, and then information about the transfer of the chemical or agent across the exposure boundaries (e.g., respiration rate, dermal permeability rate, and ingestion rate) is needed.

Generic exposure scenarios and scaling solutions

Generic exposure scenarios (GESs) represent an efficient and pragmatic solution for evaluating and communicating health and environmental risks. They identify:

- How a substance is used and how it is handled.
- What operational conditions (OCs) are typical of each of its life-cycle steps.
- What risk management measures (RMMs) are enforced.
- What potential exposures can affect the environment and workers.

Each GES contains several contributing scenarios – or default scenarios - which describe the handling activities of the substance within one life cycle step, i.e., a specific use of the substance. A substance exposure scenario (ES) describes the typical conditions under which the use of a specific substance within one life cycle step is considered safe. All these factors, along with specific predicted no effects concentration (PNEC) for environment and derived no effect level (DNEL) for human health of the substances, are required to assess risk and to calculate the risk characterization ratio (RCR).

Once the conditions for safe use have been established, the exposure scenarios are documented in a chemical safety report (CSR) and communicated down the supply chain by annexing them to the safety data sheet (SDS) to make the extended safety data sheet (ext-SDS), as required by REACH.

We can provide **generic exposure scenarios** or **scaling solutions** that match your conditions.

We provide generic exposure scenarios to our customers, for any of our products for which a GES is applicable
ExxonMobil Chemical has been at the forefront of industry efforts in this area, working closely with groups such as ESIG (ESIG on GES). As a result, our extended safety datasheets (ext-SDSs) fully incorporate the GES principles and solutions. Widely endorsed, GESs have been incorporated into the European Chemicals Agency (ECHA)'s chemical safety assessment and reporting tool (Chesar) and the CEFIC guidance on REACH exposure scenarios.

We also provide scaling solutions when our customers' use conditions are outside the GES frame
When conditions of use slightly fall outside the frame defined by the GES, there is a solution: scaling, an activity that must be carried out by the user of the substance. It is intended to determine if the exposure controls identified in the exposure scenarios (ESs) contained in ext-SDS are consistent with those being applied by the user. It identifies what actions are necessary if either the use has not been registered or local exposure control conditions differ significantly to those outlined in the GES.

If you would like to receive a GES for any of our products or more information on scaling techniques and solutions, please contact your ExxonMobil Chemical sales representatives or your distributor.

Estimate exposure

There are a variety of methods for assessing exposure for a particular situation. An **iterative or tiered approach** is often used:

- The quick screening-level technique, the lowest tier analysis
- More sophisticated techniques, usually associated with more intensive data requirements and dedicated computer models

Screening-level analysis

Screening-level analysis uses simple techniques with minimal data requirements to determine a generally conservative estimate of exposure. These assessments are conservative as they generally use reasonable worst case data inputs in the exposure calculations.

- If the exposure estimate from a screening-level assessment shows either no, or only minimal, anticipated risk, then the exposure methodology and results are reported and no further analysis is necessary.
- If the screening-level assessment exceeds acceptable criteria for exposures, then an analysis using more sophisticated exposure assessment techniques may be employed.

Simplified examples of exposure calculations for dermal, inhalation, and oral that apply to both direct and indirect methods are provided below.

Simplified examples of exposure calculations

Dermal uptake

Uptake of a substance though the skin can take place from many different environmental media, for example through contact with soil or through immersion of the skin in a liquid.
In occupational settings, immersion of the skin in a liquid is more often responsible for dermal exposure and is used in the calculation example.

A general equation for uptake for this scenario is given by:

$Uptake = (C)(SA)(K_p)(ED)(d)$	Where: Uptake:	=	dermal uptake of a chemical in water (mg)
	C	=	concentration of the chemical in water (mg/ml)
	SA	=	skin surface area exposed to the chemical (cm^2)
	K_p	=	permeability coefficient (cm/hour)
	ED	=	exposure duration (hour)
	d	=	distribution factor (1 ml of water covers 1 cm^3 on skin)

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The permeability coefficient (Kp), is one of the key variables that influences the degree to which a chemical penetrates the skin. The permeability coefficient can be measured experimentally.

Inhalation uptake

For inhalation, the intake rate is determined based upon an individual's breathing rate, or inhalation rate. The inhalation rate can vary widely depending upon many factors including an individual's level of physical exertion.

A general equation for estimating inhalation uptake is:

$ADD = \frac{(C)(IR)}{(bw)}$	Where: ADD	=	average daily dose (mg/kg/day)
	C	=	concentration (mg/m^3)
	IR	=	inhalation rate (m^3/day)
	bw	=	body weight (kg)

This simplified equation for inhalation ADD only applies as long as the substance concentration and the person's breathing rate remain constant. A more sophisticated expression for inhalation ADD will need to be applied if either of those variables changes with time.

Oral uptake

Since ingestion is not a continuous process like breathing, a slightly different model is used for estimating uptake through ingestion.

Typically, oral exposure accounts for the amount of food containing a certain substance over a defined time period, for example, one week. This is referred to as the averaging time and it should be selected so that it is consistent with the pattern of food consumption as well as the biological effect for the substance of interest.

An equation for oral uptake is:

$ADD = \frac{(C)(IR)(D)}{(bw)(AT)}$	Where: ADD	=	average daily dose (mg/kg/day)
	C	=	concentration of substance in food (mg/kg)
	IR	=	inhalation rate (kg/week)
	D	=	duration (week)
	bw	=	body weight (kg)

Occupational exposure assessment

Occupational exposure assessment (also known as occupational hygiene or occupational health management) is concerned with the prevention of health and safety hazards in the workplace and the systematic management of industrial hygiene information. The emphasis is on investigating the workplace for hazards and potential dangers as well as defining recommendations to protect the health and safety of workers and the broader community. Rigorous processes ensure products are manufactured, distributed and used safely and in a responsible manner.

Occupational exposure assessment evaluates the degree of risk when workers are exposed to chemicals in specific situations.

Recognize health hazards

Recognizing health hazards involves identifying or anticipating the nature of health risks and where they may be present in the workplace. It also includes an appraisal of any medical condition likely to increase the susceptibility of a person to hazards in the workplace.

Nature of health hazards

It is important to understand the nature of a hazard to help determine whether or not an individual is likely to be adversely affected by it. Health hazards are usually classified in 4 categories: chemical, physical, biological and ergonomic hazards.

- **Chemical hazards** include gases, vapors, dusts, mists and liquids, e.g., carbon monoxide, benzene, asbestos, welding fumes and acids.
- **Physical hazards** include noise, vibration, heat, ionizing and non-ionizing radiation and pressure.
- **Biological hazards** include bacteria, fungi, insects, animals and viruses.
- **Ergonomic hazards** are concerned with the relationship of individuals to the working environment itself and the stresses that it can cause, e.g., design of user-friendly control panels, and correct orientation of the body in relation to a task and design optimization to meet the limitations of a person.

In each case, the likelihood that a hazard will be expressed, i.e., that an adverse effect or injury will occur is related to the potential for a worker to be exposed to the hazard.

Identify the **nature** of health risks and where they may be present **in the workplace**.

Information on health hazards

Several sources of valuable information are available to anyone using ExxonMobil Chemical fluids, plasticizers and chemical intermediates and needing to identify health hazards.

- **Safety data sheets and product labels**: The hazard information for a substance is mentioned on Safety data sheets (SDS) and on product labels – as specified in REACH and GHS. Any health effects which could arise from incidental or repeated exposure to the product, as well as relevant precautions, are explained.
- **Regulation and trade body information**: Other sources of advice include the inventories of products used and guidance available from regulators or trade bodies.
- **Professional experience**: Professional experience gained from using the products is a valuable source of information. In many instances, the collective experience of groups of individuals supported by the results of medical programs provides an indication of whether a certain activity may present a health risk (i.e., the likelihood that a hazard will be expressed).

Evaluate health risks

Once the nature of a hazard has been identified, the likelihood of someone's health being adversely affected by it is determined by this individual's exposure to it. In order to evaluate whether a health risk really exists it is therefore necessary to characterize how and when exposures to it may or may not arise. There are different methods for evaluating health risks.

Formal methods of risk evaluation may be dictated by regulation. Many local regulations and directives require that health and safety risks be managed systematically. Vapor hazard ratio (VHR) and occupational exposure limits (OELs) are essential tools for evaluating whether risks to health exist in the workplace.

Exposure to a hazard

Inhalation and skin contact are the most common forms of exposure to chemicals and fluids under workplace conditions. When evaluating the health risk potential of a product, it is important to evaluate:

- the extent to which the inhalation of vapors or solids might occur
- whether skin contact might be an issue

Example: hydrocarbon fluids

When hydrocarbon fluids are used, the air in the workplace should be maintained within recommended occupational exposure limits (OELs), and if skin contact is likely, suitable gloves should be worn to prevent the material from being absorbed across the skin and into the body.

Vapor Hazard Ratio (VHR)

VHR provides a simple way to evaluate where health risks may arise during the use of volatile organic chemicals.

It assesses the tendency of a product to vaporize to its occupational exposure limit (OEL) and compares the inhalation exposure risk of fluids with different volatilities. The lower the ratio, the lower the potential risk to health.

In other words:

- a product with a high VHR represents more risk to a worker's health
- a product with a low VHR is less risky

Example: hydrocarbon fluids in industrial situations

Hydrocarbon fluids are widely used in maintenance cleaning applications. The risks to a worker's health can be significantly reduced by substituting the use of a product with a high VHR by a product with a lower VHR yet offering similar technical benefits. For products such as white spirit, significant improvements can be achieved using less volatile products possessing a lower aromatic content.

For example, Varsol™ 40 (white spirit) has a VHR of 33, compared to Isopar™ H with a VHR of 3.

Occupational Exposure Limit (OEL)

Occupational exposure limits (OELs) are values used to evaluate whether a risk to health exists in the workplace. Defined as the airborne concentration limits for a hazardous substance in the work environment, they represent concentrations below which adverse health effects can be prevented.

Most occupational exposure limits (OELs) originate from regulations established by governmental agencies or guidance from expert bodies and/or trade associations. For a list of regulatory OELs that apply in your area, you should contact your ExxonMobil Chemical sales representative.

Potential limitations

Occupational exposure limits (OELs) are valuable reference values to help manage risks from volatile substances but in order to use them properly, it is important to understand their potential limitations. Because of these limitations, it is considered best practice to maintain the concentrations of all atmospheric contaminants as far as possible below the OEL.

- **OELs serve as essential guidelines rather than a strict measure between safe and dangerous concentrations**: OELs are not simple dividing lines between safe and dangerous concentrations. They represent concentrations at which adverse health effects should not arise in most people when exposed to specified substances on a daily basis. This means that a substance may still be smelled (and appear unpleasant to some people) or may cause low level effects, such as irritation, in some people. It also means that short term exposures above the OEL often have no health consequence. OELs therefore serve as essential guidelines in the process of evaluating and controlling potentially hazardous substances.
- **An OEL is subject to review**: An OEL represents the best assessment of the available scientific information at the time it was established. It should not be seen as permanent value and is subject to review as new data becomes available.

OELs for ExxonMobil Chemical fluids: reciprocal calculation procedure (RCP)

ExxonMobil Chemical has also developed its own OELs to support its range of products. They are the company's equivalent of the American Conference of Governmental Hygienists (ACGIH) Threshold Limit Values (TLVs).

Hydrocarbon fluids, broadly used in industrial applications, are either mono-constituent substances or complex hydrocarbon substances containing multiple components. Whilst OELs are available for many substances, few have been established for complex hydrocarbon fluids. Furthermore where regulatory bodies have established OELs for some common complex hydrocarbon fluids, this has not been achieved on a consistent basis. Typical examples are the OELs for different definitions of white spirit in certain countries.

Since 2000 ExxonMobil Chemical has been developing its own OELs, using the Reciprocal Calculation Procedure (RCP). The method is in line with the approach used by the American Conference of Governmental Hygienists (ACGIH).

The RCP derives an OEL based upon the relative proportion of hydrocarbon fluid components and their respective OELs. The procedure covers aliphatics, aromatics and cycloalkanes in the range C5-C20. It is only applicable for airborne exposure to vapors. Its application has not yet been established for halogenated or oxygenated hydrocarbons and exposure to mists or via skin contact is outside its scope.

In principle the RCP requires an OEL for each component of a complex hydrocarbon fluid but to be practical, when constituents have similar physical, chemical and toxicological properties, they may be grouped and a single value (group guidance value or GGV) identified to cover a number of constituents. However, some specific hydrocarbon solvent constituents such as n-hexane have unique toxicological properties and are included in the RCP calculation using their unique exposure limit values (Specific Substance Values or SSVs).

The RCP method was also adopted by the European Hydrocarbon Solvent producers Association (HSPA) in 1999 for use by its members to calculate OELs for complex hydrocarbon solvents for inclusion in their safety data sheets. A paper recommending GGVs and SSVs encompassing all hydrocarbon solvent constituents was published in 2005 (McKee et al., 2005), and the method was then adopted by the U.S. ACGIH (2008).

ExxonMobil Chemical's approach
ExxonMobil Chemical's OELs refer to exposures for an 8-hour day, 40-hour working week, except where otherwise stated. If adverse effects may arise from short term exposures, then specific short term exposure limits are given.

These OELs are developed by a committee made up of senior ExxonMobil Chemical experts in toxicology, industrial hygiene and epidemiology. As with other OELs systems, ExxonMobil Chemical gives priority to valid human data over those from animals testing. Where there are no human data, then the OEL is derived from available animal data or by analogy with similar chemicals possessing an established regulatory OEL.

Together, the regulatory OELs and ExxonMobil OELs form a sound basis for a consistent standard of protection for workers.

Derived No Effect Level (DNEL)
A similar but somewhat different approach to characterizing hazards of substances to workers and the general population was introduced by the EU REACH regulation.

The regulation requires that information on substances (physicochemical properties, environmental and toxicological data) be compiled and evaluated and a No Observed Adverse Effect Level (NOAEL) be determined based on results from toxicology tests. The NOAEL is then used in the calculation of the Derived No Effect Level (DNEL) through the application of certain adjustment factors. In this context the DNEL is a level which is "safe", i.e., a level below which the expression of hazards is not expected. The DNEL is then compared to the level of exposure anticipated when using the substance.

Simply put, if the exposure estimate is below the DNEL, the use is considered to be safe. If the exposure estimate exceeds the DNEL, then actions are required which could include closer assessment of the exposure estimates or recommendations for additional exposure control measures (see following sections).

ExxonMobil developed DNELs for its EU REACH-registered products. This information was part of the EU REACH registration requirements and is available via the ECHA website.

OELs vs. DNELs
Both Derived No Effect Levels (DNELs) and Occupational Exposure Limits (OELs) play a critical role in the human health risk characterization process. However, it should be noted that although there are similarities between the two, they are not exactly the same and do not have precisely the same purposes.

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DNEL: an OEL as defined by EU REACH

A DNEL represents a safe dose, that is a level of exposure to a substance at or under which human exposure is safe in defined usage conditions. DNELs are calculated from the results of toxicology studies or other relevant information following a methodology established within the EU REACH registration guidelines, and they are used as a benchmark to assess whether or not exposures associated with different uses are potentially problematic

OEL

OELS are exposure concentrations under which it is believed that nearly all workers may be repeatedly exposed, day after day, over a working lifetime, without adverse effect. An OEL represents the maximum concentration of a substance in workplace air that a worker can be exposed to, based on an 8 hour time weighted average. In some cases, short term fifteen minute exposure limits are established.
An OEL may be derived from the same initial data but often incorporates an integrated peer analysis of toxicological, epidemiological, clinical, sampling and analytical method sensitivity in the scientific determination. The OEL typically carries regulatory authority aimed to prevent over-exposure in the workplace.

In fact the DNELs and OELs for fluids are similar because they are derived from the same data but they are not precisely the same because of the methodological differences in derivation.

Occupational hygiene evaluation

When health issues are identified, exposure assessment or monitoring may be required to evaluate risks.

Quantify the exposure

Various methods of evaluation may be used to quantify exposure to health hazards. Sampling may be required over a time period, e.g., a working shift or the duration of a particular task. The evaluation may be repeated to improve the confidence in the results.

Qualify the exposure

Other methods of evaluation may be qualitatively determined based on professional experience. For example, exposure risks while using household products such as bleaches, paint strippers or garden chemicals can be assessed by exposure science professionals based on experience, knowledge and published information. Similarly, informal studies may take place on the work premises.

Occupational hygiene monitoring vs. OELs or DNELs

The results of occupational hygiene monitoring are often compared with available occupational exposure limits (OELs) or other values such as DNELs. It is important that these measurements are accurate and conform to relevant national requirements. There are a number of national and international sampling and analytical methods promulgated by relevant governmental and industry bodies.

It is important to consult an industrial hygiene professional to select a method that is most appropriate to the specific situation at hand.

ECETOC TRA 3

Developing and promoting quality science, ECETOC is the leading European scientific forum for the ecotoxicology and toxicology of chemicals, biomaterials and pharmaceuticals. ECETOC is an independent organisation, highly-respected in the regulatory and scientific communities. Founded in 1978 and based in Brussels, ECETOC's work focuses on the health assessment and environmental safety of substances.

ECETOC's Targeted Risk Assessment (TRA) tool consists of three separate models for estimating exposures to workers, consumers and the environment that arise during a series of events (exposure scenarios). It has been identified by the European Commission's Regulation on Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) as a preferred approach for evaluating consumer and worker health risks.

Control risks to health

Different types of controls are used on a daily basis to reduce or eliminate health risks. Some are built into chemical processes or work activities, others are introduced at a later stage as a result of experience or formal assessment.

Control strategies may require changes to work practices or control devices to be used in a certain way. It is therefore critical that the workforce is educated and trained to the new measures in place. It is also important that local factors, ranging from technical constraints to functionality and cost, are considered as well.

A number of options are available to control risks to health:

Elimination
Eliminate the use of hazardous substance at the development stage of a new product or process is the ideal solution for control, but is often technically impractical.

Substitution
Substitution is about replacing a contaminating substance, activity or process with a less toxic alternative or installing a better process to reduce the health risk.

Examples include:

- Replacing Exxsol™ Hexane with Exxsol™ Isohexane
- Choosing 'low-dusting' ingredients when solids must be frequently handled manually (e.g., in the form of pellets or flakes)
- Using vacuum cleaners rather than brushes for sweeping and cleaning areas contaminated with hazardous dusts.
- Knowing the vapor hazard ratio (VHR) of a product when choosing fluids for different applications. If possible, choose a product with a low VHR.

Limit specification
A limit may be specified on the content of very toxic materials in products in order to reduce health risks. Some products are regulated in this manner, for example:

- Legislation prohibits certain potent carcinogens not to exceed a certain threshold in marketed products.
- Similar "toxic thresholds" exist for other classes of materials, e.g., sensitizers, where they must be clearly labeled for the degree of hazard they present.

Manufacturers and users of products may also introduce specifications which limit the quantity of a material within a product.

Beware that limiting health risks this way require a reputable supplier to operate a credible quality control scheme. In the absence of such quality control schemes on the supplier's part, purchasers should check product specifications using in-house quality control systems.

Ventilation

Different methods of ventilation are applicable to different situations.

Dilution ventilation

Dilution ventilation is the dilution of contaminated air with clean air to maintain contaminants at acceptable levels. However, this technique, while reducing the level of contamination in one area, can spread it at low levels to other areas where individuals may be present and contaminate them.

Local exhaust ventilation

Local exhaust ventilation captures and controls airborne releases at or close to the point of emission by means of ventilation that transports the contaminant to a point where it can be safely collected or discharged.

This type of ventilation is particularly valuable for situations requiring the identification of the release point for the contaminant. It minimizes contamination of the workplace, and captured polluted air can be more readily treated.

Consulting an industrial ventilation expert for further advice on the control of exposure to workplace contaminants by means of ventilation is highly recommended.

Exposure limitation

Limit the exposure of workers by restricting access to a risk area, in terms of the time they spend or their proximity to the hazard, provided that the exposure remains within the acceptable levels.

Engineering controls

Engineering controls such as enclosing activities is a common method of reducing health risks, although may not be an option in some cases, e.g., during maintenance.

Personal Protective Equipment

In the workplace, personal protection can be achieved by means of:

- Eye protection (e.g., safety glasses)
- Skin protection (e.g., gloves, gauntlets)
- Foot protection (safety shoes and boots)
- Respiratory protection (e.g., masks and respirators)
- Protective clothing

Many authorities consider personal protection equipment (PPE) to be the least preferable form of control, but in practice it is commonly used, for example:

- For maintenance tasks or where other forms of control do not offer complete protection, e.g., when connecting or disconnecting pipelines.
- Allows flexibility in protecting, based on route of exposure concern over a range of conditions.

Unfortunately, many studies have shown that the protection offered in practice is often far lower than intended by suppliers due to inappropriate use of the equipment. It is important to ensure personnel are knowledgeable on the proper selection, use and limitations of their PPE.

International standards

Different international standards govern the performance testing of PPE. They ensure users can rely on a consistent product from different suppliers but they do not guarantee the product will adequately perform in practice.

Proper selection of equipment and training of users

Effectiveness of a control solution is also a function of the proper selection of PPE and the training of users. A critical aspect is choosing adequate materials of construction for protective clothing.

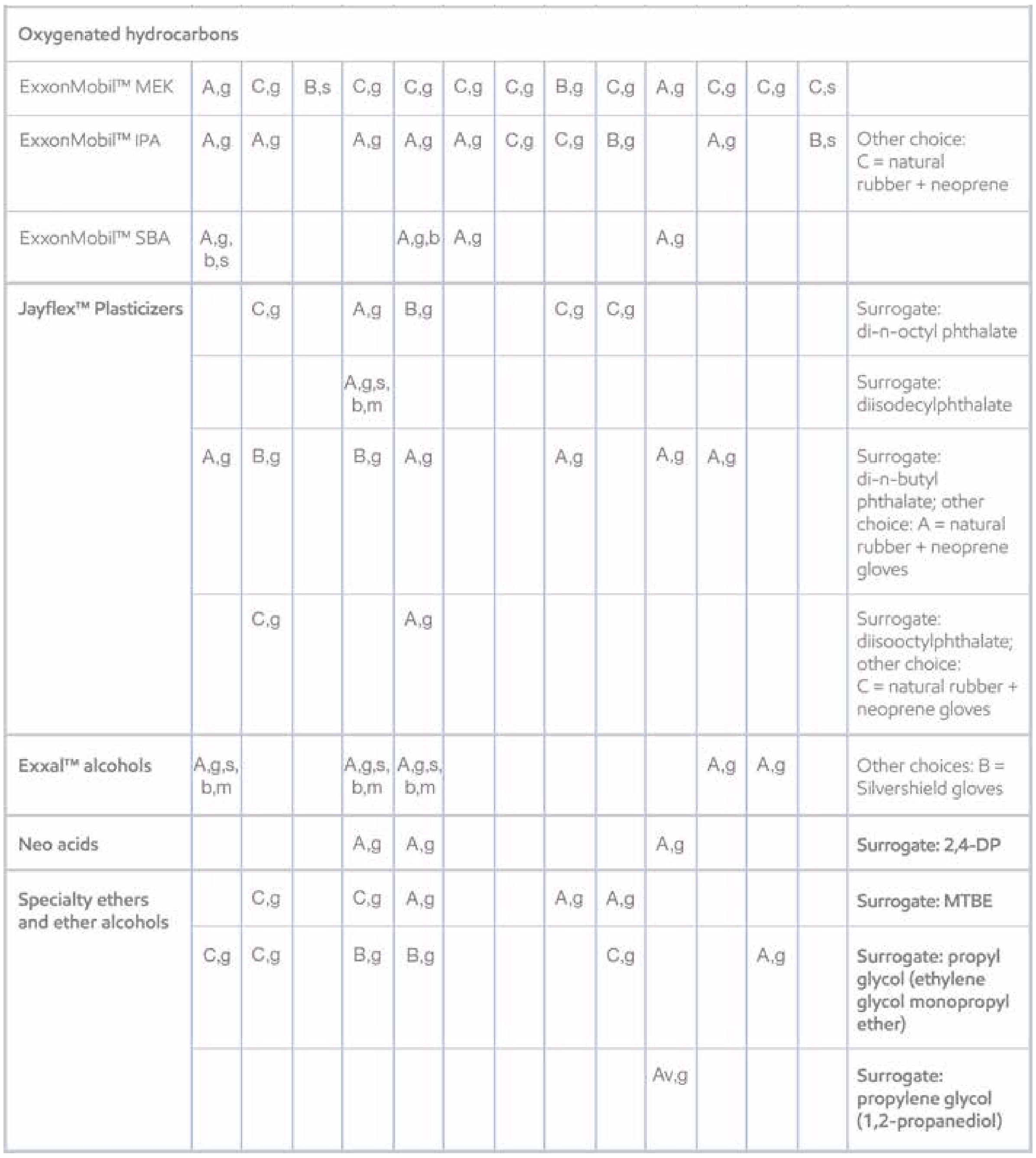
Choice of materials of construction for protective clothing

When choosing personal protective clothing, the manufacturer's data should be respected to make sure that the equipment is compatible with the working conditions and the substance being handled. It should be impervious to the contaminant or, at the very least, offer a reasonable degree of permeation (penetration) resistance.

The table below uses chemicals similar ('surrogates') to ExxonMobil Chemical's for which data is available and relevant.

Barrier material	Butyl Rubber	Natural Rubber	Butyl/Neoprene	Neoprene	Nitrile	Nitrile/PVC	Polyethylene	Polyvinyl Alcohol	PVC	4H (PE/EVAL/PE)	Viton	Viton/Neoprene	Saranex	Barrier material
ExxonMobil Product														Comments
Aliphatic and alicyclic hydrocarbons (Exxsol™; Isopar™; Norpar; Exx-print™)	C,g,s	C,g		A,g	A,g		A,g	A,g	A,g,s		A,g			Surrogate: kerosene
Aromatic hydrocarbons														
Solvent Toluene	C,g, s,m	C,g		C,g,b	C,g	C,g,b	C,g,c	A,g	C,g, b,c	A,g	A,g	B,g,s	C,s	Other choice: A = Viton/chlorbutyl suits
Solvesso™					B,g,s, b,m					B,g	A,g			Other choices: B = Silvershield
Nappar™ ranges	C,g,s	C,g		B,g	A,g		A,g	A,g	A,g,s		A,g			Surrogate: naphtha <3% aromatics (b.p. 150-200°C)
HAN					B,g,s, b,m					B,g	A,g	A,g		Other choices: B = Silvershield glove
Aromatic/Aliphatic hydrocarbons (Varsol™; Exx-print)	C,g	C,g		B,g	A,g		C,c	B,g	C,g	A,g			A,s	Surrogates: mineral spirits; stoddard solvent

Codes		
A	=	Provides effective barrier against repeated exposures over a work shift
B	=	Provides effective barrier in limited testing or effective against certain specific chemicals in class, i.e., protection against splashes or limited exposure.
C	=	Provides little or no protection against chemical penetration other than those listed.
c	=	coveralls
g	=	gloves
s	=	suits
b	=	boots
m	=	miscellaneous types of garments other than those listed.



Oxygenated hydrocarbons														
ExxonMobil™ MEK	A,g	C,g	B,s	C,g	C,g	C,g	C,g	B,g	C,g	A,g	C,g	C,g	C,s	
ExxonMobil™ IPA	A,g	A,g		A,g	A,g	A,g	C,g	C,g	B,g		A,g		B,s	Other choice: C = natural rubber + neoprene
ExxonMobil™ SBA	A,g, b,s				A,g,b	A,g				A,g				
Jayflex™ Plasticizers		C,g		A,g	B,g			C,g	C,g					Surrogate: di-n-octyl phthalate
				A,g,s, b,m										Surrogate: diisodecylphthalate
	A,g	B,g		B,g	A,g			A,g		A,g	A,g			Surrogate: di-n-butyl phthalate; other choice: A = natural rubber + neoprene gloves
		C,g			A,g									Surrogate: diisooctylphthalate; other choice: C = natural rubber + neoprene gloves
Exxal™ alcohols	A,g,s, b,m			A,g,s, b,m	A,g,s, b,m						A,g	A,g		Other choices: B = Silvershield gloves
Neo acids				A,g	A,g					A,g				**Surrogate: 2,4-DP**
Specialty ethers and ether alcohols		C,g		C,g	A,g			A,g	A,g					**Surrogate: MTBE**
	C,g	C,g		B,g	B,g				C,g			A,g		**Surrogate: propyl glycol (ethylene glycol monopropyl ether)**
										Av,g				**Surrogate: propylene glycol (1,2-propanediol)**

Codes		
A	=	Provides effective barrier against repeated exposures over a work shift
B	=	Provides effective barrier in limited testing or effective against certain specific chemicals in class, i.e., protection against splashes or limited exposure.
C	=	Provides little or no protection against chemical penetration other than those listed.
c	=	coveralls
g	=	gloves
s	=	suits
b	=	boots
m	=	miscellaneous types of garments other than those listed.

Note that the information referring to specific PPE products or materials should not be considered as an endorsement by ExxonMobil or ExxonMobil Biomedical Sciences, Inc. or its affiliates on their use. The PPE selection information supplied is based on manufacturer supplied permeation data as reported in the reference databases.

Respiratory Protective Equipment

In the workplace, the lungs are the quickest route for the entry of materials into the body. When airborne exposures to hazardous substances are not adequately controlled, it may be relevant to consider respiratory protection.

Respiratory protection equipment (RPE) has an important role but should still only be considered when it is impractical to control the risk in other ways, i.e., through engineering controls or substitution.

Criteria for suitable equipment

The type of respiratory protective equipment (RPE) used will depend on the type of contaminant anticipated, whether it is a solid (e.g., powder) or a gas/vapor. Many different types of respirators are available, with specifications and designs offering varying levels of protection, so that choosing the right equipment is critical.

An RPE device is suitable if it provides appropriate protection for a given application.

- Fit the person it is intended for, taking personal factors into account, e.g., facial size, facial hair.
- Be capable of providing the appropriate protection, e.g., use of correct filters, where applicable.
- Be matched to the task. For example, it must not hinder vision or mobility, nor impose excessive or inappropriate physiological burdens on the wearer. Special assessment may be needed for wearers with medical conditions.
- Be compatible with any other items of personal protection equipment (PPE), e.g., eye, hearing and/or skin protection, and not impede the level of protection provided by such PPE.
- Not cause or unduly exacerbate physiological stresses such as heat stress.
- Provide suitable protection for the entire duration of the task.

The selection of the correct respiratory protection requires a detailed knowledge of the nature of workplace exposures and of the capabilities and limitations of available respiratory protection. Maintenance systems must be installed to support the continued performance of the protection over time.

Unfortunately, respirators are often seen as a cheap alternative to engineering controls and over time, their operating costs are often substantial.

Further technical information is available from RPE manufacturers.

Minimum protection factor

The minimum factor by which the concentration of contaminant in the workplace must be reduced to reach an acceptable level helps determine if the RPE is adequate.

Respiratory Protection Equipment (RPE) is considered adequate if it provides a suitable and sufficient level of protection to reduce the exposure of the wearer to an acceptable level, relative to the appropriate Occupational Exposure Limit (OEL).

To determine if the RPE is adequate, it is necessary to calculate the minimum factor by which the concentration of contaminant in the workplace must be reduced to reach an acceptable level, that is well below an applicable OEL (i.e., such as OES, MEL, MAK, TLV or ExxonMobil Chemical OELs). It is the factor that determines the minimum required protection factor of the RPE, and is defined by various key institutions such as OSHA, NIOSH, or sometimes by local regulation.

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Calculation of the Protection Factor (PF):

- Workplace concentration outside the face piece (e.g., breathing mask) of the RPE
- Maximum allowable concentration inside the face piece of the RPE

PF is sometimes also expressed as:

- Workplace contaminant concentration outside the RPE
- Workplace contaminant concentration inside the RPE

Leakage is a significant factor
The protection factor of any given RPE is significantly dependent on the level of inward or outward leakage of the RPE. Leakage will vary according to the quality of fit, flow rate (if applicable), training and expertise of the wearer, as well as factors as such temperature, humidity, maintenance, and the conditions of use.

Minimum protection factor vs. nominal protection factor:
In many areas, the minimum protection factor is preferred to the former Nominal Protection Factors (NPFs) based on the minimum acceptable performance in laboratory tests.

Assigned protection factor
The assigned protection factor, derived from RPE product performance and workplace exposure data, is considered a good basis for evaluating the performance of RPE.

In the case RPE is not used properly, its performance may not match its original performance specifications. Assigned protection factors (APFs) are used to reflect actual usage protection performance.

Derived from RPE product performance and workplace exposure data, AFPs more realistically reflect true levels of exposure in actual usage. They are considered to offer health and safety professionals a more reliable indicator of the level of protection offered by different types of RPE.

APFs are defined as the minimum expected workplace level of RPE that would be provided by a properly functioning respirator, or class of respirators, to a stated percentage of properly fitted and trained users (e.g., typically, 95%). In many cases, they are guidance values rather than absolute values.

It should also be particularly noted that APF values for different RPE types will vary according to the national organizations and institutions. For example, key bodies such as NIOSH recommend that users always select the RPE type with the highest APF that is compatible with the conditions of each particular workplace, especially with respect to carcinogens.

It is therefore essential that RPE users consult their national guidelines for determining which APFs are applicable to different RPE types.

Maintenance of control measures
Most of the systems and equipment used to control exposure deteriorate over time.
The performance of ventilation systems and respirators declines with normal wear and tear.
An enclosed system remains contained only if leaks do not occur from valves or shafts.
This means that regular checks need to be made to ensure continued performance.

Planned maintenance should be carried out on critical items against key performance criteria derived from satisfactory performance of the control:

- For a ventilation system, this may mean measuring extraction velocities or system efficiencies at key locations at regular intervals.
- For a respirator or breathing device, it might require checks to be made on the condition of valves, seals and securing straps.

Occasional checks should be carried out on individuals too, in order to ensure that they are adhering to work practices designed to reduce exposure. Routine industrial hygiene monitoring should be carried out to show that control measures, such as ventilation, perform to a desired specification or to pinpoint areas for further improvement.

Manage risks to health

Occupational hygiene is as much dependent on effective management systems which support health objectives as it is on the occupational hygiene principles themselves.

The overall objective of ensuring that adverse health effects do not arise in exposed populations, including consumers and the community, demands that industrial hygiene performance is monitored and that suitable cross-functional systems are available. Such systems involve:

- Defining relevant objectives and supporting targets.
- Assigning an organizational framework with responsibilities for action.
- Establishing appropriate systems and procedures which enable the objectives to be delivered.
- Verifying progress and performance against the overall objectives and supporting targets.
- Incorporating a process of feedback and review.

A **successful** occupational health management program needs **managerial commitment**.

An occupational hygiene program cannot succeed without managerial commitment and additional systems which support and complement the overall objective, such as:

- Inspection and maintenance of control measures
- Adoption and enforcement of recognized (e.g., ExxonMobil Chemical's) OELs in helping to demonstrate that risks to health are adequately controlled
- Workplace medical programs (or health surveillance) that can evaluate levels of exposure or other adverse health effects in people. Health monitoring serves as a performance indicator.

Legislation incorporates similar principles for the broader management of all workplace health and safety issues.

Consumer exposure assessment

Consumer exposure assessment evaluates exposures to the general population from contact with a wide range of consumer products. A consumer product is any material or substance that is used in a non-occupational environment.

Complex patterns of exposure

Consumer exposure assessment is often more complex than occupational exposure assessments owing to more complex patterns of exposure, the greater number of microenvironments visited, and the longer periods of time available for exposures to potentially occur compared to an 8-hour work shift.

In some instances, consumers may be subjected to higher levels of exposure than a worker who has proper controls in place. Consumer exposures can be greater than those experienced in the workplace for a particular substance since safeguards to protect an individual, such as proper ventilation or appropriate personal protective equipment (PPE) may not be available or may not be used. In addition, the consumer is often in close proximity to the source of the exposure, that is, the consumer product. Generally, the closer one is to the source, the greater the exposure can be.

In part due to the complexity of the exposure scenarios for consumer products, exposure assessors have come to rely on specialized exposure models to estimate consumer exposures. One of the main purposes of this type of model is to integrate the exposures one might experience to a particular substance from multiple sources and potentially through multiple routes of exposure, during a defined exposure period.

> The **complexity** of consumer exposure assessment has led to the development of **specialized exposure models**.

Consumer exposure models

A number of modeling tools are developed to assess consumer exposures and evaluate appropriate hazard/risk levels associated with specific products/uses. Nevertheless, there still is, in general, limited available data on exposure factors for consumers.

- **ESIG** has developed a GES consumer tool that enables users to develop their own consumer Chemical Safety Assessment/Exposure Scenario (CSA/ES) for a particular area of use that can be based upon the results of the various communication and use mapping activities that have been undertaken with major Downstream User (DU) groups.
- **Consumer Exposure Model** (CONSEXPO) **developed by RIVM in the Netherlands**
  An example of a consumer exposure model is the Consumer Exposure Model (CONSEXPO) developed by RIVM in the Netherlands. The CONSEXPO model is a multi-route human exposure model accounting for exposures by the inhalation, ingestion, and dermal routes. In addition, it has the capability to estimate uptake separately for all three routes of exposure.
- **The U.S. Environmental Protection Agency's Exposure and Fate Assessment Screening Tool, also called** E-Fast2. Another example of a consumer exposure model is the U.S. Environmental Protection Agency's Exposure and Fate Assessment Screening Tool, also called E-Fast2.

The Consumer Exposure Module (CEM) is an interactive model within E-FAST2 that calculates conservative estimates of potential inhalation exposure, and potential and absorbed dermal exposure to chemicals in certain types of consumer products. The CEM allows screening-level estimates of potential acute dose rates, potential peak concentrations, and potential lifetime average daily concentrations and doses.

Community exposure assessment

Community exposure assessment is applicable to people who are not industry employees and assesses their exposure to hazards that are neither a result of direct contact with consumer products nor a result of exposure to the hazard associated with their work.

Examples of community exposure are:

- Inhalation of direct emissions outside a facility's fence line
- Ingestion of a substance that moved through the environment before ultimately accumulating in groundwater used as a source of drinking water

The latter scenario is sometimes referred to as an indirect exposure because the contact with the substance does not directly occur after release from a source. The substance can move from one environmental "compartment" (e.g., air, soil, surface water) to one or more other compartments before coming into contact with people. This can greatly increase the complexity of the exposure assessment beyond that for occupational exposures and even those for consumer exposures.

Modeling tools

Various modeling tools have been developed to help determine potential exposures to a community. The tools can be grouped into two general categories:

- Those that estimate the concentration of a substance in the environment
- Those that estimate the actual exposure to individuals

The former method predicts the environmental concentration of a substance which must then be combined with additional information such as exposure factors to estimate the resulting exposures.

Examples of models which estimate concentrations in air are:

- The Atmospheric Dispersion Modeling System (ADMS) developed in the United Kingdom
- The AMS/EPA Regulatory Model (AERMOD) developed jointly by the American Meteorological Society and the U.S. Environmental Protection Agency
- The U.S. EPA's Total Risk Integrated Methodology (TRIM)

AERMOD and TRIM combine the prediction of environmental concentrations with the additional information needed to estimate exposure into a single modeling platform. They are complex and require extensive input data to calculate community exposures.

Predicted environmental concentrations (PECs) of a substance

As an alternative to modeling, an assessor may use predicted environmental concentrations of a substance, when available, to determine exposures.

The estimated concentration of a chemical in a particular place, or medium, at a particular location and time, is called the predicted environmental concentration (PEC).

Determining a PEC and then relating it to a No Observed Adverse Effect Level (NOAEL) (or another acceptable no-effect level in humans for non-cancer effects) is a common method of prioritizing the potential risks posed by actual exposures to chemicals.

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VOCs and indoor air quality

Indoor air quality can play a significant role in health, especially for individuals who spend a substantial amount of time indoors – at home or at work. While indoor air quality may be impacted by outdoor air, most indoor air pollutants are generated or released indoors.

Indoor air recommendations for the general public may differ from occupational recommendations for professionals because sources of indoor air pollutants, level of exposures, and duration of exposures typically differ.

Elements affecting indoor air quality »

Personal, physical, biological and chemical factors can all impact the well-being of a person in an indoor environment.

Potential health effects »

Indoor air pollutants can cause health problems such as respiratory illnesses or allergies. The health effects may be immediate, from a single or repeated exposures, or may occur after long-term exposures.

Impact of ExxonMobil products on indoor air quality »

The impact of ExxonMobil Chemical fluids, plasticizers and chemical intermediates on the quality of the air that people breathe at home.

VOCs and indoor air quality regulations »

There is currently a lack of a common definition of indoor air quality and legislation in this area is emerging and will develop in the future.

Elements affecting indoor air quality

A multitude of personal, physical, biological and chemical factors impact the well-being of a person in an indoor environment. It is therefore important to recognize that the chemical factor is only one of them and that it is necessary to address the issue of indoor air quality with an integrated approach.

Chemicals that release VOCs

Chemicals used for household cleaning and maintenance, personal care, and hobbies may all contribute to indoor air pollution. For example:

- Window cleaning products may contain glycols.
- Adhesives may contain ketones and hydrocarbon solvents.
- Paints and air fresheners may contain hydrocarbon and oxygenated solvents.
- Dearomatized fluids may be used in aerosol formulations.

These products may release volatile organic compounds (VOCs) into the indoor environment during use. They represent substances with diverse characteristics and properties and may be categorized as VOCs but they are typically grouped together when evaluating their impact on indoor air quality.

Indoor air quality is impacted by many different factors and should be considered with an **integrated approach**.

Other common sources of VOCs

Other common sources of VOCs in indoor air are tobacco smoke, paint strippers, varnishes, waxes, personal care products (aerosols), ozone generating devices, cleaning and disinfecting chemicals, solvents and degreasers, and furnishings such as fabrics and pressed wood furniture. Some air fresheners, deodorizers and fragrances may also contribute to VOCs in indoor air. Exposures to VOCs from routine consumer use are generally low when products are used as directed, however elevated exposures may occur with misuse.

When assessing indoor air quality, the full range of potential emission sources should be considered. For example: carbon monoxide, pesticides, dry cleaning chemicals, particles and fibers, such as combustion products, asbestos and lead, microorganisms, animals and insects.

Indoor environmental factors

Indoor environmental factors can impact generation, accumulation, and overall impact of these sources:

- **High temperatures** can increase the concentration of some indoor air pollutants, especially VOCs as elevated temperature will drive evaporation.
- **Humidity** in indoor air should be controlled to optimize human comfort and minimize indoor air quality issues. Most experts recommend between 30 and 70% humidity in indoor air.
- **Personal activities** can also release air pollutants, intermittently or continuously. There are many examples: smoking, cooking, air fresheners, nail polish and hair sprays, hobbies that use glues, varnishes, paints or solvents, etc.

- **Ventilation** is one of the most important factors in indoor air quality. Adequate ventilation is necessary to dilute emissions from indoor sources and to carry pollutants out of the building. Some current recommendations can be found through the following organizations:

  - Commission of the European Communities
  - European Committee for Standardization
  - ASHRAE, American Society of Heating, Refrigeration, and Air-Conditioning Engineers

Potential health effects

The real impact of pollutants found in indoor air on health is not clear yet as many factors may come into play, such as the level of product concentrations, periods of exposure, interpersonal variability, respect of use instructions, etc. Further research is needed.

While VOCs are typically grouped together in indoor air quality research, only a subset of these substances has been linked to adverse health effects. Several studies show a link between the use of some consumer products and adverse health effects. However, it is not clear to what extent pollutants are solely responsible for the observed effects because other factors may also contribute. In addition, it is also unclear as to whether use instructions were properly followed in studies where effects were observed. Further research is needed to better understand potential links between specific or mixtures of indoor air pollutants and specific health effects.

> Further research is needed to **assess the real health impact** of pollutants found in indoor air.

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Elements affecting indoor air quality

Potential health effects

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Impact of ExxonMobil products on indoor air quality

The impact of ExxonMobil Chemical fluids, plasticizers and chemical intermediates on the quality of the air that people breathe at home.

Plasticizers found in vinyl products such as vinyl flooring, window and tile sealants (caulks), clothing, and children's toys (excluding toys than can be placed in the mouth), may contain high molecular weight phthalates such as DINP (di-isononyl phthalate) and DIDP (di-isodecyl phthalate). Due to their low volatility, high molecular weight phthalates are not typically found in indoor air.

> Regulators conclude that there are no risks to adults or children from the use of DINP and DIDP in current flexible PVC applications.

High molecular weight phthalates have been measured in house dust. This can be related to abraded particles of flexible PVC from, for example, flooring and footwear. The phthalates in these abraded particles and phthalates adsorbed to dust particles are not normally biologically available and hence are not absorbed. Studies have shown that there is no correlation between levels of phthalates in dust and human exposure. Human biomonitoring studies show that exposure to high molecular weight phthalates of consumers is well within safe limits. Regulators have used these and other data to conclude that there are no risks to adults or children from the use of DINP and DIDP in current flexible PVC applications.

VOCs and indoor air quality regulations

Due to the multitude of factors that can impact our health in an indoor environment and the multiple combinations of physical, biological, chemical and personal factors that come into play, it is important to address the issue of indoor air quality with an integrated approach.

Furthermore, the general population's exposure to air quality should be considered at two levels:

- Direct, from exposure to volatile products in the workplace or from the use of consumer products at home;
- Indirect, when associated with exposure conditions from professional uses, e.g., the exposure of persons to solvents in a house repainted by professionals.

Because of this complexity, regulators are addressing the topic of indoor air quality gradually, with an objective to reduce the amount of polluting emissions and control air quality.

Main regulations and standards in Europe

- Construction product regulation: EU 2011/305
- It lays down harmonized conditions for the marketing of construction products in Europe.
- European Solvents Coordination Group (ES-VOC-CG): paper on VOCs and indoor air quality
- ECO-label indoor outdoor paints and varnishes CD 2009/544/EC
- It establishes the ecological criteria for the award of the Community eco-label to indoor paints and varnishes.
- ECO-label indoor outdoor paints and varnishes CD 2009/543/EC
- It establishes the ecological criteria for the award of the Community eco-label to outdoor paints and varnishes.

In the U.S. and Asia Pacific, indoor air quality regulations are developing.

Environment

Scientific advancements and new legislation continue to drive the development of environmental toxicology, or ecotoxicology, and fate assessment. In this section, we introduce the basics of ecotoxicology and present the different methods and tests in place to analyze substances and determine their toxicity and fate in the aquatic, terrestrial and air media.

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Basics of ecotoxicology

The study of ecotoxicology is devoted to understanding the causal links between exposure to chemicals and possible changes to ecosystems. It draws from two broad fields:

- Ecology, or the study of ecosystems and the interactions of organisms within it; and
- Toxicology, or the study of the biological effects caused by physical, chemical or biological agents.

Key concepts »

Key concepts such as ecotoxicity, ecosystem, and environmental fate processes are critical to the understanding of ecotoxicology.

Physicochemical properties of substances »

The physicochemical properties of substances determine their behavior in different conditions and their impact on the environment.

Standardized laboratory testing »

Standardized laboratory testing provides the controlled conditions necessary to establish cause and effect relationships between exposure concentration and biological effects.

Key concepts

A few concepts are important in the understanding of ecotoxicology.

Ecosystem

An ecosystem consists of both non-living (e.g., soil, air, water, nutrients) and living (e.g., animals, bacteria, plants) components. Each is defined in terms of its structure and function and is affected by a number of factors.

Structure

The ecosystem structure refers to the composition of the components (i.e., the different organism populations and habitats that need to be protected).

Function

The ecosystem function focuses on the role these components play in contributing to the overall health of the system (e.g., nutrient cycling, energy flow).

Modifying factors

Numerous natural and man-made factors can alter the ecosystem structure or function:

- Natural factors, such as climate, inter-species competition, natural succession, etc.
- Man-made factors, such as habitat loss, exotic species introduction, agricultural-, fisheries- and wildlife management policies, etc.

Exposure

The concentration of the substance to which the organisms are exposed is the most important parameter to control. In order to relate effects to exposure, a constant, known exposure concentration for a specific period of time is required. As the effect is related to the internal dose the organisms receive, exposure durations need to be long enough to ensure sufficient uptake of the chemical by the test organism.

Different variables can affect toxicity results. They can be physical effects that impact exposure or relate to the different routes of exposure.

Physical effects can cause unrealistic exposures due to the method by which the test substance is introduced into the test system (e.g., emulsions of undissolved substances in aqueous test media). Under these circumstances, small organisms such as water fleas (Daphnia magna) may become coated with an undissolved test substance and die from suffocation. Care must be taken, especially when testing with poorly water soluble substances, which includes many petrochemical products, to avoid physical effects that could result in an erroneous hazard interpretation.

Metabolism results in the biochemical transformation of the test substance into other compounds which facilitates excretion.

Transformation process: biodegradation

To characterize the transformation processes, standardized tests have been defined to allow some prediction of the degradability of chemical substances in the environment. These are generally divided into tests of abiotic degradation (or chemical degradation) and tests of biodegradability.

Biodegradability

Microorganisms may chemically modify a substance in a variety of ways, all of which could be considered biodegradation. The type and number of organisms are as important to the outcome of the biodegradation process as the structure of the chemical. This is also one of the reasons for the variability observed in biodegradation experiments.

The different types of biodegradation have been classified according to:

The extent of the modification

- A simple structural change in the parent substance or primary biodegradation
- Complete degradation to carbon dioxide or ultimate biodegradation.

The results of the "extent of the modification" testing for ExxonMobil Chemical fluids, plasticizers and chemical intermediates are available on request.

Influence of the environment on biodegradation

The microorganisms (bacteria) which accomplish the biodegradation are most important to the nature of the result. Generally, the interest in studying biodegradation is to use the results to predict the environmental fate of a chemical (its biodegradability).

As a result, the microorganisms used in laboratory tests are naturally occurring mixtures of species (as opposed to single, pure strains) taken from a particular environment. For a variety of reasons, sewage sludge has come to be the standard source of mixed microorganisms for introduction into laboratory biodegradation test systems (the inoculum). In marine biodegradation tests, however, the natural microorganism community present in field collected seawater is used.

Certain environmental conditions, such as availability of oxygen, greatly influence the types of organisms and their metabolic pathways. Laboratory tests under conditions of no oxygen (i.e., anaerobic) have also been standardized. Some factors influencing biodegradation results are shown in the table.

Other, more specific, environmental conditions have also been defined for biodegradation in soil, sea water, and sewage treatment systems. Biodegradation tests intended to exactly replicate organisms, their environment, and their exposure to the chemical are called simulation tests.

Factors affecting biodegradation	
Organism related variables	Species present (competence and diversity)
	Population density (concentration)
	Prior conditions (adaptation and acclimation)
	Spatial distribution
Substrate related variables	Concentration
	Solubility/bioavailability
	Structure ("biodegradability")
	Other chemicals present (co-metabolism, inhibition)
	Toxicity
Environment related variables	Oxygen availability
	Nutrients (nitrogen, phosphorous)
	Temperature
	pH

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Factors affecting biodegradation	
Environment related variables	Mixing/turbulence
	Salinity
	Moisture (soil)

Rate of biodegradation
The rate of biodegradation reflects the growth rate of organisms under the conditions of the test, whether in the aquatic environment or in a standardized laboratory test.

In the aquatic environment, bacteria are exposed to low concentrations of a variety of chemicals and nutrients that they use to maintain rather stable populations.

In the standardized laboratory tests of biodegradability, the organisms are constrained within a small volume of water and presented with a high concentration of the test substance as the sole source of carbon.

Some organisms degrade the chemical, using it as both the source of carbon for new cells (biomass) and energy, and therefore grow as they degrade. The rate of this biodegradation reflects the growth rate of those particular organisms under the conditions of the test. The kinetics are therefore completely defined by the test and are not easily related to rates in the environment.

Ready biodegradability
Standardized test guidelines are developed, validated, and used for regulatory purposes to evaluate both the rate and extent of biodegradation.

Test requirement/criteria for ready biodegradability
Tests to assess the ready biodegradability of substances (e.g., their ability to biodegrade rapidly) use sewage treatment plant microorganisms which have not been previously exposed (adapted) to the chemical. Ultimate biodegradation, or complete mineralization of the test substance, can be measured as carbon dioxide (CO2) production, oxygen (O2) consumption, oxygen utilization, or dissolved organic carbon (DOC) disappearance is the endpoint in these tests. In order to be characterized as "readily biodegradable", a substance must meet the criterion of 60% degradation through CO2 or O2 measurement or 70% through DOC measurement within 28 days. A further stipulation, referred to as a 10-day window, requires that the pass criteria must be met within 10 days after biodegradation exceeds 10%.

Interpretation of results
The different analyses give different results. Disappearance of the DOC is more rapid than the utilization of oxygen or the production of CO2.
Ready biodegradation tests are considered so stringent that if a substance meets the criteria to pass a test, it will also rapidly degrade under most aerobic environmental conditions. Further, given the acknowledged range in variability of degradation by the sludge microorganisms, a substance will be considered to be readily biodegradable if it meets the criteria to pass only one test. So, if data from five tests are available, and one of the five shows the substance to be readily biodegradable, then the substance is considered to be so. This is accepted by regulatory authorities.

In addition, if a substance does not pass a ready test, it does not necessarily mean that it would not degrade in the environment. Rather, further data such as simulation tests, are needed to better characterize biodegradation under more realistic conditions.

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A variety of analytical methods

A number of ready biodegradability tests are available and each one dictates the procedure and the applicability of the test for different types of substances:

- Manometric respirometry is most relevant for volatile and/or poorly soluble substances and for ExxonMobil Chemical hydrocarbon and oxygenated fluids.
- The CO_2 test (or "modified Sturm" test) uses an air flow through the test flask to collect CO_2 and hence cannot be used for volatile substances.
- The die-away test uses DOC disappearance for analysis and hence cannot be used for poorly soluble substances.
- The Closed Bottle test is applicable for volatile substances, but uses a lower initial biomass than the other ready tests due to the limitation in oxygen solubility

Comparing biodegradation test results

There are numerous pitfalls in the comparison of the results of biodegradability tests for the same or similar products. As a consequence, the variability of results imply that the comparison of biodegradability between substances is only truly quantitative if tested in the same test systems using the same inoculum prepared at the same time. The major use of biodegradation tests is therefore merely to provide an estimate of the potential of a substance to degrade in the environment.
The main reasons for variations are:

Variability in appropriate tests

There can be significant variations coming from different factors, for example:

- Even within tests of the same type, the inoculum can make a difference in the outcome of the test.
- The initial number of competent organisms affects the duration of the lag phase (or adaptation phase). If the number of competent organisms in sewage sludge is low, different tests could show either good biodegradation or minimal.
- The content of microorganisms in the inoculum source may vary over time, so that even the standard inoculum will give much more variability in biodegradation tests than in physical property or even toxicity tests.

Use of inappropriate tests

Another common pitfall in biodegradation testing is the use of an inappropriate test:

- If a material is highly adsorbing or becomes insoluble during the test, then tests based on DOC disappearance will give a falsely high biodegradability.
- Tests of volatile substances in open systems will give too low a result if the analysis is CO_2 or O_2, and falsely high results if the analysis is DOC because the evaporated chemical is not accounted for.
- Toxicity of the chemical may lead to low results, particularly in tests which use high concentrations (for instance MITI).
- Other deviations from standardized conditions can influence the result, such as higher or lower temperature and presence or absence of other nutrients.

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Types of regulatory biodegradation tests

An overview of the biodegradation tests and their specific quantitative definitions within certain standardized tests

Types of biodegradation tests

Attribute	Categories	Measurement	Properties
Extent	Ultimate	0_2, CO_2, DOC (Dissolved Organic Carbon)	Measures total conversion to inorganic forms (e.g., CO_2, H_2O, etc.), mineralisation
	Primary	Specific analysis	Based on analysis of specific chemical or chemical class, abiotic losses controlled
	Removal		Primary, both abiotic & biodegradation
Ease	Ready	DOC, 0_2, CO_2	Regulatory definition of 'rapid' biodegradability uses < 30 mg/l non-adapted inoculum, reaches minimum 60% (0_2 or CO_2) or 70% (DOC) in 28 days and must go from 10% to 50% in 10 days
	Inherent	High biomass, adapted	Enhanced conditions to show possibility to eventually biodegrade
	Simulation	Specific environments	Reflects actual environmental behaviour but difficult to simulate most actual exposures

Biodegradation test results

Most of the ExxonMobil Chemical fluids (hydrocarbon and oxygenated) are readily or inherently biodegradable per the appropriate OECD test methodology. For additional information on the testing results please contact ExxonMobil Chemical.

Aromatic hydrocarbons vs. paraffins

Aromatic hydrocarbon solvents tend to be slightly more soluble and give better results in standardized tests than paraffinic solvents. Among the paraffins, the normal, or linear, molecules are considered more biodegradable. This is due to the fact that the biodegradation process involves microbial oxidation of one end of the linear molecule to a carboxylic acid. The resultant fatty acid is easily further degraded by a normal metabolic process present in nearly all organisms.

Complex hydrocarbon substances: ThOD vs. COD

Using the Theoretical Oxygen Demand (ThOD) as the denominator of the biodegradation equation is useful when calculating complex hydrocarbon substance biodegradation.
In comparison, the poor performance of the Chemical Oxygen Demand (COD) methodology, which is normally used for undefined or variable mixtures, can result in false biodegradation results. Use of COD may result in falsely low oxygen demand, which in turn results in false biodegradation results.

The presence of branching somewhat hinders degradation. For volatile hydrocarbons, much of the older data made use of the Closed Bottle test, an unstirred test system with lower inoculum. As a consequence, these substances were often thought not to be readily biodegradable per OECD testing.

Most ExxonMobil Chemical plasticizers and chemical intermediates are readily or inherently biodegradable per OECD testing. Exceptions are the ExxonMobil neo acid grades which contain quaternary carbon structures. Quaternary carbon structures enhance the stability of chemicals, which can be a beneficial property for some product applications. The higher olefins are also not readily biodegradable due to the high degree of branching inherent in these substances. For additional information please contact ExxonMobil Chemical.

Toxicity in the environment

Ecotoxicity assessment defines the capacity of a substance to affect environmental species, populations or ecosystems. Potential hazards to the environment are assessed, followed by assessment of exposure to the potential hazards. Risk is a function of both hazard and exposure, both of which are necessary in order for there to be risk.

Hazard vs. risk

The distinction between the terms hazard and risk is important.

- Hazard refers to the inherent capacity of a substance to cause an adverse effect.
- Risk is the actual likelihood that the hazard will occur in the real world, based on potential or expected exposures.

Thus, a product can pose an environmental hazard under exposure conditions achieved in laboratory toxicity tests, but not constitute an environmental risk if such exposures are never achieved in the aquatic environment.

Environmental fate

Assessing environmental fate determines what happens to a substance if it is released into the environment: physicochemical properties are important considerations in determining which of the different media the substance will end up in.

Primary and secondary media

Broadly speaking, the environment can be divided into primary and secondary media, each of which has several compartments:

- Primary media, e.g., air, water, soil, sediment
- Secondary media, e.g., plants, other organisms

> Assessing environmental fate determines **what happens to a substance** if it is released into the environment.

Distribution and concentration of a substance

A fate assessment describes the distribution and concentration of a substance in the various environmental compartments as a function of time and distance from the point of release into the environment. The assessment begins by considering the substance emissions to air, water, soil and sediment during substance life cycle including production, transport, industrial use, consumer use and disposal. Emissions to these primary media can be from multiple sources, and can be considered on a local and regional (large) scale.

Transport, transformation and accumulation of a substance

Once released into the environment, a substance follows a series of evolutionary processes that determine its ultimate environmental fate:

- Transport, for example through advection, dispersion, partitioning, etc.
- Transformation, such as abiotic degradation and biotic degradation,
- Accumulation, e.g., bioaccumulation in secondary media such as plants and organisms.

Testing

Laboratory tests or predictive methods which can characterize relevant physicochemical properties and fate processes are critical elements needed for environmental fate assessments.

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Physicochemical properties of substances

The properties of chemicals will dictate their effect on the environment and their ability to affect living organisms in various environmental compartments. They will also be responsible for the chemicals' ultimate fate, persistency, assimilation or bioaccumulation.

A number of physicochemical property measurements are relevant to the environmental behavior of substances.

Some of them are routinely measured in the chemical industry. However, the use of the data for calculation of the environmental fate of components of complex substances (such as many hydrocarbon products) often requires more detailed information about the range of properties.

Chemical structure

The properties of chemicals depend upon their chemical structure, that is their molecular structure and carbon number.

ExxonMobil Chemical fluids
ExxonMobil Chemical fluids may have a number of hydrocarbon structures with a range of molecular weights and chemical types, so knowledge of the relative composition becomes important.

ExxonMobil Chemical fluids differ within each family by a progression in boiling point ranges, which indicates a similar progression in the number of carbon atoms in the product. Depending on the family considered, there are differences in the breadth of the range, but generally, for these fluid products, the carbon number ranges are narrow: 5-carbons or less.

Jayflex™ plasticizers, Exxal™ alcohols and ExxonMobil™ neo acids
Jayflex™ plasticizers, Exxal™ alcohols and ExxonMobil™ neo acids are characterized by components with a common functional group (alcohol, acid, ester, etc.)

These products have a narrow range of carbon numbers, thus can have a more narrow range of physicochemical properties than the fluids. Consequently, physical properties for a representative isomer in these products can often be used to assess environmental fate of the product itself.

Physicochemical properties of environmental importance

Table summarizing the physical property measurements relevant to the environmental behavior of substances.

Physical Property	Definition	Environmental importance (Regulatory use)
Chemical Structure	**Molecular weight (range), formula, functional groups, branching, etc.**	**Determines other physical and chemical properties (QSARs, particularly K_{ow})**
Octanol/water partition coefficient[1] (K_{ow})	Equilibrium concentration ratio between octanol and water	Determines partitioning to lipid in organisms, sludge, soil (QSAR estimates of toxicity, partitioning, water solubility)
Vapour Pressure[1] (VP)	Partial pressure of vapour	Determines tendency to leave liquid state and become gas, enter air. (Estimation of evaporation and volatilisation rates and extent)
Water Solubility[1]	Aqueous concentration at saturation	Determines extent to which it will dissolve. (Estimate water concentrations, volatility)
Soil [organic] partition coefficient (K_d[K_{oc}])	Equilibrium concentration between soil and water	Determines tendency to stick (sorb) to particles. (Estimation of mobility through soil, sorption to sediment, toxicity in soil)
Dissociation Constant (K_a)	Ionisation of acids or bases	Ionisation extent at environmental pH influences other properties. (Estimation of effective concentration)
Melting and Boiling Points[1] (MP and BP)	Critical temperatures for phase changes: solid - liquid - gas	Physical form in the environment. (Related to VP & solubility)

[1] A range of values would be appropriate for complex substances (mixtures)

Octanol/water partition coefficient

The K_{ow} is an important indicator of the lipophilicity of a substance, e.g., its relative affinity to lipids (fats) rather than water. The K_{ow} is used in many different predictive models, including those for toxicity and bioaccumulation.

Relationship between octanol and water solubility

The measure of hydrophobicity of a substance is an important physicochemical property for environmental fate, bioaccumulation and toxicity modeling. To experimentally derive the Kow, the test substance is placed in a vessel containing a layer of octanol and a layer of water; the two are not miscible. In this test system, octanol is meant to act as a representative for fat (or lipid), such as that in a fish swimming in a pond. The test measures the tendency of the test substance to partition to octanol (fish fat/lipid) versus water. The importance of this partitioning has been recognized since the early 1900s through work by Meyer and Overton showing that the narcotic potency of chemicals was closely related to oil/water partitioning behavior in a large series of experiments with different exposure routes and several different animals and plants.

> The K_{ow} indicates the **lipophilicity of a substance** and is used in predictive models for **toxicity and bioaccumulation.**

Methods for determining K_{ow}

- The slow-stirring method employs a temperature-controlled vessel, in which octanol, water, and test substance are allowed to equilibrate with gentle stirring to accelerate the process. After equilibrium is reached, the water and octanol phases are separated and analyzed for substance concentration. The ratio of concentrations in octanol to water is the K_{ow}. KOW = octanol/water
- The shake-flask method has been widely used, wherein an aqueous solution of the substance is mixed with octanol in a vessel, which is agitated or shaken, to facilitate equilibration of substance between the two phases. The water and octanol phases are separated and analyzed for substance concentration. The ratio of concentrations in octanol to water is the K_{ow}. The HPLC (high pressure liquid chromatography) method measures the retention time of the substance on a hydrophobic HPLC column and compares it with the retention times of a number of standards with known K_{ow} values.

It is also possible to estimate K_{OW} using one of several different computer models based on structure-activity relationships.

Due to the wide range of measured values, Kow is usually expressed as the logarithm (Log K_{ow} or Log P_{ow}). Log K_{ow} values are generally inversely related to aqueous solubility.

ExxonMobil Chemical fluids

Simple hydrocarbon components have measured values for Kow which are reported in the literature, but due to the complexity of many ExxonMobil Chemical fluids, selecting a single K_{ow} for these substances is not possible. While simple hydrocarbons provide an indication of the K_{ow} of the typical substances found in complex products, variations occur between chemical classes:

- At the same carbon number, aromatic substances have a lower K_{ow} than aliphatic substances
- Linear (normal) paraffins have slightly higher Kow values than the corresponding branched (iso) paraffins or cyclic paraffins (naphthenics)

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- ExxonMobil Chemical fluids generally contain hydrocarbons with log K_{ow} values over 3.0 and many of the heavier materials have components with log Kow values greater than 6.0, indicating high hydrophobicity.
- Some of the oxygenated fluids are exceptions: these oxygen-containing molecules are more polar than hydrocarbons. For example, IPA, MEK and SBA all have log Kow values lower than 1
- Within a chemical class, the Kow increases in proportion to the carbon number.

ExxonMobil Chemical plasticizers and chemical intermediates

- The acids (ExxonMobil™ neo acids) and the alcohols (Exxal™ alcohols) generally have log K_{ow} values lower than 3.0
- The esters (Jayflex™ plasticizers) have high log K_{ow} values, generally above 7.0
- Within a chemical class, the K_{ow} increases in proportion to the carbon number.

Physicochemical properties of environmental importance

Water solubility

The aquatic fate and effects of a substance are highly dependent upon its solubility in water. The measurement of water solubility can be straightforward, by progressively adding the substance to water and analyzing the water until saturation is reached.

However, substances with different physical properties (liquid and complex substances) require specifically adapted methods to determine their water solubility.

Liquid substances with low water solubility

The analysis must be specific to the substance to prevent interference from more water-soluble contaminants. For substances of very low water solubility, a slow-stir method is used wherein the test substance is carefully added to water. This is gently stirred to avoid forming emulsions. The water is analyzed for the substance until equilibrium has been reached. This method is best suited to liquid substances. In the absence of measured data, a number of QSAR-based computer models are available to estimate water solubility based on chemical structure.

> The aquatic fate of substances depend a lot on their solubility in water. For complex substances, it is a complicated process.

Complex substances

For complex substances, such as ExxonMobil Chemical hydrocarbon fluids, individual components in the product have different water solubilities which makes it impossible to define the solubility of the mixture. Once the least soluble component saturates the water, an undissolved phase begins to form. The remaining components will partition between the water and the undissolved phase. The composition of the water extract will therefore be different to the composition of the neat substance.

The behavior of complex substances makes it impossible to define solubility and complicates the conduct and interpretation of aquatic toxicity tests. The lighter, aromatic-containing hydrocarbons have components with solubility above 1 mg/L, but in general most hydrocarbon fluid components have water solubility below 1 mg/L.

Physicochemical properties of environmental importance

Vapor pressure and volatility

The vapor pressure (VP) is a measure of substance solubility in air. VP is important for determining both the rate of evaporation and relative amount of the substance that will be in the air phase. Within a given substance class, vapor pressure tends to decrease with increasing molecular weight.

Physicochemical properties of environmental importance

Henry's law constant and volatility

Henry's law constant (HLC) indicates the relative partitioning of a substance between air and water. It is an important parameter in estimating the degree and rate of volatilization of a substance from water into air. It may be directly measured analytically within a test system or, more commonly, taken as the ratio of the vapor pressure (Pa) to the molar water solubility. The HLC is expressed in units of Pa - m3/mole.

The low water solubility and relatively high vapor pressures of hydrocarbons results in high HLC values. Generally, an HLC value of 10 Pa-m3/mole or higher indicates that volatilization is a significant fate process for the chemical.

Hydrocarbon fluids
Hydrocarbon fluids are particularly likely to volatilize from water, more so for paraffins than aromatics, which have somewhat higher water solubilities:

- The solubility of most substances decreases faster than vapor pressure with increasing molecular weight, so that HLC values increase with increasing molecular weight.
- For large molecules, the vapor pressures become too low for volatilization to be an important fate process. This is the case with some of the higher molecular weight range hydrocarbon fluids grades.

ExxonMobil Chemical fluids
For complex substances such as ExxonMobil Chemical fluids, each component has differing water solubilities and vapor pressures, so the HLC value may cover a wide range.

Jayflex™ plasticizers, Exxal™ alcohols and ExxonMobil™ neo acids
For many chemical intermediates and plasticizers, a reliable HLC is difficult to determine due to the low vapor pressure and aqueous solubility of these products.

Physicochemical properties of environmental importance

Adsorption and desorption

Adsorption is the transfer of a gas, vapor or dissolved material to the surface of a solid. Desorption is the reverse process. The adsorption of organic chemicals from water to sediment or soil plays an important role in fate modeling. This process is also important in exposure modeling for aquatic organisms, sediment-dwelling organisms and soil organisms. Soil/water equilibrium also has a determining influence on the mobility of chemicals in ground water.

At the screening level, the test procedure involves overnight mixing of the chemical in solution with added soil. A variety of soil types are used. After this equilibration, the soil is separated and placed in pure water. Specific analyses of the water phases are made to determine the extent of adsorption and desorption. If the test substance is adsorbed (> 25%) and not easily desorbed (< 75%), then more thorough investigation of the kinetics and concentration dependency of the adsorption is required. The concentration behavior is not always a simple linear relationship and is described as an isotherm.

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However, for most modeling applications the assumption of a constant distribution coefficient between soil and water (K_d) is sufficient.

For un-ionized substances, it has been shown that the important determinant for adsorption is the organic matter content of the soil, so the results for various soils are normalized by calculating the partitioning coefficient between water and soil organic matter (K_{oc}). The K_{oc} is often directly calculated from the K_{ow}.

Physicochemical properties of environmental importance

Dissociation constant (pKa)

Some chemical substances dissociate into ionic forms in the aquatic environment. This dissociation greatly influences their environmental fate, since the ionic form tends not to partition into air or non-polar environmental media like soil or sediment.

The ionic species also have different aquatic toxicity from the unionized form. Most commonly, acid or base equilibrium is involved wherein, for example, an acid loses a hydrogen ion and forms an anion. The methods used to establish the equilibrium concentration of ionized and unionized forms is generally simple titration for acids or bases. For **substances of low water solubility**, spectrophotometric methods may be used.

Neo acids are weak carboxylic acids which are expected to be more than 90% in the ionized form at neutral pHs. Since the ionized form is generally less toxic to aquatic life, this dissociation behavior explains why this class exhibits low aquatic toxicity.

Physicochemical properties of environmental importance

Standardized laboratory testing

Laboratory testing with single species is a critical tool for ecotoxicity assessments. Tests vary in the species utilized, the duration over which chemical exposure occurs and the endpoints used to characterize environmental hazards.

Controlled lab conditions

The most realistic way to evaluate the effect of chemicals on the environment might seem to be through field studies. In reality, laboratories are a better environment to establish cause and effect relationships between the exposure concentration and the biological effects because effects of chemicals are best studied under controlled conditions.

Limitations of field studies
It is very difficult to quantitatively evaluate the level of harm associated with the magnitude of the release of a substance in field studies. This is because the concentration of the substance to which organisms are exposed (or exposure concentration) is continuously changing due to different factors:

- Diffusion away from the point of release
- Movement to other media (i.e., transport between soil, water, sediment and air)
- Movement of the organism within the plume (as in plume of smoke) of substance in the test media from a point of release
- Adsorption of the substance in soil and sediment
- Degradation (both biological and physical) of the substance
- Natural cycles impacting populations of organisms, and physical conditions such as rainfall or high levels of sunshine
- Presence of other contaminants in the environment

> The biological effects of chemicals are **best studied in laboratories, under controlled conditions**.

Test populations and species
In standardized toxicity tests, populations are selected to improve the reproducibility of test results and their relative comparison. The selection is based on reduced biological variability and single test species, which is critical to achieve meaningful ecotoxicity assessments:

- Organisms of the same age range, similar in size, and in good health with no observable abnormalities are used.
- Differing species sensitivities are addressed by testing representative species from various levels in the food chain (trophic levels).
- Organisms used in testing are generally bred in the test laboratory, but may be purchased from outside sources.

By using representative species, substances tested at different times may be compared for relative toxicity. Quantitative structure-activity relationships (QSARs) developed for specific species and based on structural or physical properties of the substances, have a good predictability of toxicity, especially in the aquatic environment.

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More details on controlled lab conditions

Examples of organisms commonly used in ecotoxicity tests

The table below lists several common aquatic and terrestrial test species that have been used in toxicity tests. Species are selected for a variety of reasons, including historical use, ease of culture and relevance to the region in which the testing is being done. This list is not all-inclusive.

Environmental Media	Organisms
Aquatic	Bacteria (Vibrio fischeri)
	Algae (green, red, brown)
	Crustaceans (daphnia, shrimp, mysids)
	Fish (e.g., rainbow trout, zebrafish, Japanese medaka, fathead minnows, bluegill, guppy)
Benthic (sediment-dwelling)	Crustaceans (amphipods)
	Insects (midge)
	Worms (oligochaetes)
Terrestrial (soil dwelling)	Plants (e.g., lettuce, radish, rye grass)
	Worms (earthworms, oligochaetes)
	Collembola

Aquatic tests in static, static-renewal or flow-through conditions

Exposure in aquatic toxicity tests may be described as static, static-renewal or flow-through conditions and reported as nominal (as prepared or calculated) or measured (by chemical analysis) concentrations. The type of exposure condition required depends upon the stability of the test chemical in the aqueous exposure media. If chemical concentrations remain relatively constant over the exposure period, static tests may be used. However, if chemical concentrations change appreciably over the test duration, periodic (static) renewal or flow-through conditions are usually used. In certain cases, a pulsed exposure rather than a constant exposure may be used better to simulate exposure concentrations under real world conditions (e.g., accidental spill).

Environmental variables

Environmental variables may modify toxicity by competing with, or influencing the form of the toxicant under investigation.
Examples:

- The aquatic toxicity of metals and organic acids are dependent upon water quality parameters such as hardness and pH.
- The ecotoxicity of non-polar organic chemicals in soils and sediments depends upon the organic carbon content of these solids.

Depending on the conditions, test organisms will therefore react differently and the chemical properties of the substances will be impacted.

Quantitative relationships

Laboratory toxicity tests provide a basis for a quantitative relationship between the exposure concentration and the resulting biological effects, and a consistent way to evaluate environmental hazards. This is achieved by testing individual components in separate, carefully controlled laboratory test systems:

- Physicochemical properties, if necessary
- Substance degradation rates under specific conditions
- The toxicity to organisms, under controlled exposure and conditions

Chemical comparisons and read-across

The standardization of laboratory testing generally allows for the comparison of the relative toxicity of different substances in the same species, as the test conditions are all the same. Such comparisons have led to the development of scientific relationships between the physicochemical and biological properties of test substances.
For example, when a homologous series of chemicals is tested, such as alcohols of increasing carbon chain length, there is a fairly continuous change in some physicochemical properties and toxicity. This uniform, predictable change may be used to infer the result for untested members of the series. This process is often referred to as read-across.

Extrapolation to the environment

Controlled laboratory test results can be used as part of the risk assessment process:

- Tests of physical properties, degradation rates and toxicity may be used to indicate the potential fate and effects of the substance in the environment under a variety of conditions and exposures.
- The transportation properties and degradation rates may be combined in mathematical models to calculate the exposure concentrations.
- The concentration-response relationship is used to estimate the environmental effects.

The most commonly employed ecotoxicity tests performed in laboratories are aquatic tests. Terrestrial tests are conducted under certain conditions only. The impact of volatile organic compounds (VOCs) on air is a more recent area of research.

Exposure and tests

Constant exposure concentration and duration are critical to enable significant comparisons in toxicity testing.

Although relatively easy to achieve with stable and water soluble products, this is a real technical challenge for other categories of products such as substances with low water solubility or volatile substances.

Stable, water soluble chemicals

Typically, a series of exposure concentrations is tested, often in a logarithmic progression. Test guidelines require that the actual concentration be confirmed analytically over the course of the exposure. The resulting data from this test allows the determination of an accurate concentration-response curve.

From this data, the median lethal concentration (LC50) is statistically derived. This is the concentration that will theoretically kill 50% of the organisms in the test.

For other acute endpoints not involving lethality, the median lethal effect EC50 is used to indicate effect concentration rather than lethal concentration.

For chronic endpoints other than lethality - such as effects on growth or reproduction - statistics are used to derive no observed effects concentrations (NOEC), or EC10 values. NOEC refers to the highest exposure concentration in a chronic test that does not statistically differ from control organisms. An EC10 is a concentration that will cause effect in 10% of the test organisms.

It should be noted that the direction of the concentration-effect relationship is such that if a substance has an effect at a lower concentration than another it has a higher toxicity.

Volatile or unstable substances

For volatile or unstable substances, ensuring that exposure concentrations are reasonably constant over the entire duration of the test is difficult. There are a few approaches to address this issue:

- Replace static exposure concentrations with frequent renewal of the exposure medium with freshly prepared test solution.
- Use a continuous flow of test solution through the exposure chambers (flow-through tests).
- Prevent loss by testing in tightly closed containers (with care to ensure that organisms get sufficient oxygen).

The purpose of these tests is to produce a quantitative concentration-response relationship, not to simulate the fate and effects of the substance in the environment. So the expected (nominal) concentration must be confirmed with chemical analysis.

Substances with low water solubility

Low water solubility substances, such as many petrochemical products, must be carefully tested so that the concentration of exposure during a test is maintained stable. This allows for accurate determination of effect concentrations. Knowledge on accurate test substance concentrations and variability is often lacking in historical tests.

Solubility cut-off

Substances with low water solubility will generally have greater toxicity than more water soluble substances. However, as the number of carbon atoms in the series increases, the water solubility decreases, usually more so than the toxicity increases. A point will be reached when no effects are evident. This is sometimes referred to as the solubility cut-off. Further additions of a simple substance above its solubility limit will not increase the dissolved portion which is absorbable by the test organisms, and therefore is not bioavailable.

Low water solubility substances must be **tested very carefully** and **exposure concentration** maintained stable during the test.

Limit test: a standard test

Sometimes tests are conducted as limit tests in which the substance is added in an amount greater than its solubility to meet arbitrary toxicity limits, such as 100 mg/L. In this example, if there is no effect at the limit concentration, the result may be reported as LC0 (EC0,or LL0) as 100 mg/L and the substance is considered to have minimal toxicity. An alternative, if less than 50% mortality is observed, the LC50 (or EC50 or LL50) may be reported as >100 mg/L.There are two potential sources of error inherent in this approach:

- The presence of minor components which are water soluble may affect the results. At additions above the water solubility of the main substance, the contaminants may continue to dissolve and may constitute a higher percentage of the water solution than the substance itself. In these cases, the toxicity observed may be erroneously ascribed to the main substance. It is recommended to use high purity test substances.
- Another potential error involves the occurrence of physical effects of the undissolved test material. Such effects may become confused with the chemical toxicity of the bioavailable portion. Examples of such problems are the fouling of fish gills by oil droplets which can cause suffocation, as well as surface entrapment of daphnia in a surface film of a chemical, causing immobility (the endpoint in daphnia acute toxicity tests).

Addition of emulsifiers or solvents

In some cases, emulsifiers or solvents are used to generate a homogeneous dispersion of low soluble substances into water. There should be no effects observed due to emulsifiers. However, if large amounts of such materials are used, the test substance may supersaturate the system with artificially high concentrations. This is often observed when testing substances with very low water solubility.

There are concerns with this approach as it distorts the environmental conditions prevailing in the test system and may significantly alter the test results. It is recommended to avoid using emulsifiers or solvents in aquatic toxicity testing. If emulsifiers or solvents are used, care should be taken to ensure that the concentrations achieved during the test do not exceed the aqueous solubility of the test substance.

Complex substances

ExxonMobil™ hydrocarbon fluids are complex substances generally composed of low water soluble substances, a number of which are also very volatile. Specific tests are designed to minimize the challenges caused by these substances' inherent properties.

Water solubility and lethal loading

For complex products of low water soluble substances, each individual component may have a different water solubility. Consequently, with the addition of increasing mass of the substance to water, complex equilibria are established between the individual compounds making the insoluble chemical component phase (usually floating on the surface) and the water. These equilibria will vary with the mass of substance added.

As a result, additions of a complex substance to water at levels beyond the water solubility of the components results in a solution and a toxicity measurement which no longer accurately reflects the composition or toxicity of the complete substance.

> **Lethal loading** is the test methodology that provides the toxicity data used in **classifying danger** to the aquatic environment for **complex, low solubility substances**.

This test methodology bases the toxicity measurement on the amount of substance added to water and not the concentration of the dissolved components. The amount of substance added has been dubbed the loading, and is not the same as the nominal concentration since:

- The substance is generally not completely dissolved
- The dissolved fraction is different in composition from the substance
- The composition of the dissolved fraction changes with the loading and often different components predominate at different loadings

The toxicity values derived from such tests are often described as LL50 (or EL50) for median lethal loading (or median effect loading) to distinguish the results from tests on soluble, simple substances (LC50 or E5C0).

The portion of substance which separates after equilibration is generally removed leaving behind the aqueous phase, is referred to as the WAF (water accommodated fraction). Dilutions of the WAF should not be used for testing. Instead, individual WAFs are prepared at different product loadings. This allows for the realistic equilibria that vary with loading, giving a result that is relevant to environmental situations. For example, if a spill occurs, it will not be of a concentrated water extract of the substance, but comprise the whole of the substance at rather low substance to water ratios.

LL50 data allows an immediate quantitative assessment of how much substance in a given volume of water is likely to result in toxicity and is the appropriate toxicity data to use in classifying danger to the aquatic environment for complex, low solubility substances.

Volatility and closed systems
Some ExxonMobil Chemical products have high volatility. It is therefore necessary to test in closed systems with very close attention to minimizing any air spaces or losses to air of volatile components either in performing the test or in preparing the WAF.

Modeling: QSARs

A number of methods are used to determine correlations and extrapolate test results. A widely used tool is quantitative structure-activity relationships (QSAR).

Quantitative structure-activity relationships models
Quantitative structure-activity relationships models, or QSARs, are predictive models that derive correlations between physicochemical properties and biological activities of test substances. In other words, they are methods for estimating properties of a chemical from its molecular structure and have the potential to provide information on hazards of chemicals, while reducing time, monetary cost and animal testing currently needed.

The use of QSAR estimates has become valuable information in global risk assessment processes, to evaluate the reliability of measured data and to substitute for missing data.

Example:
An accepted relationship is that between the lipophilicity of a substance (as measured by octanol/ water partition coefficient, K_{ow}) and water solubility (high K_{ow} correlates with low water solubility), soil sorption (high K_{ow} correlates with high soil sorption), and toxicity (increasing KOW correlates with increasing toxicity).

Please click here for more information on QSARs.

Test endpoints

Ecotoxicity test endpoints are usually divided into acute and chronic:

- Acute endpoints generally involve gross adverse effects (e.g., mortality or immobilization) determined over a short segment of the test organism lifespan.
- Chronic tests typically focus on more subtle, sub-lethal effects (e.g., growth or reproduction) determined over a longer period of test organism life cycle.

A comparison of the different attributes of acute and chronic toxicity tests

A comparison of acute and chronic ecotoxicity tests

Test	Acute	Chronic
Objective	determines test material concentration that causes effect on organism during short term exposure	designed to determine lowest observable effect and no observable effect concentrations of a material
	evaluates relative toxicity of different materials to same organism	
	valuates relative sensitivity of different species to same material	
Onset of effect	sudden or delayed	delayed
Concentration of test material	relatively high	relatively low
Exposure frequency	continuous or pulsed	continuous or pulsed
Test duration	typically ≤ 4 days	weeks, months
	exposure short compared to life cycle (egg to adult) of organism	may include entire life cycle of organism
Effect typically measured	mortality	development
	immobilisation	animal growth
	algal growth	reproduction

Toxicity and fate in the aquatic environment

The understanding of the toxicity and fate of substances in the environment is critical for environmental risk assessment. Toxicity (essentially chronic and sub-chronic levels) and fate in the environment (refers to the processes that a substance goes through when released in the environment) are determined by a series of various tests.

Aquatic toxicity »

A series of different tests are performed to determine the different levels of ecotoxicity of substances – essentially acute and chronic toxicity.

Fate in the aquatic environment »

A presentation of the three main processes that a substance entering the aquatic environment goes through: transport, transformation and bioaccumulation.

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Aquatic toxicity

Different tests are performed to determine the acute and chronic levels of ecotoxicity.

Testing for acute aquatic toxicity

Acute endpoints generally involve gross adverse effects (e.g., mortality or immobilization) determined over a short segment of the test organism lifespan.

The general approach to all toxicity tests is to expose organisms to a series of concentrations of the test substance. The species used in tests – algae, invertebrates (such as the Daphnia magna) and fish – are typical representatives of plants, invertebrates and vertebrates that are part of the food chain.

The concentrations are chosen, often based on preliminary tests, so that the biological effect (e.g., mortality) occurs over the range of concentrations. At the lowest concentration, little to no effect is ideally observed while at the highest concentration the effect is maximal.

Acute aquatic toxicity tests

The intention is to provide testing at different levels within the aquatic food web. Algae, invertebrates, and fish are generally included in the aquatic testing scheme. Acute toxicity tests on these three levels of organisms are a general requirement for meeting global regulatory data requirements for the aquatic environment.

A variety of species have been identified which are used as standard test organisms in these studies. Nevertheless, marine organisms may have different responses to toxicants: the intent is to have surrogate species which are easy to culture and breed in the laboratory, are relatively sensitive to toxicity, and are well-studied so that their responses may be readily interpreted. These species are intended to be a conservative representation of the entire aquatic environment. The species most generally selected for freshwater toxicity tests are the rainbow trout *Oncorhynchus mykiss* (fish, OECD 203), Daphnia magna (invertebrate, OECD 202), and *Pseudokirchneriella subcapitata* (green algae, OECD 201).

Data resulting from toxicity tests are generally used to calculate the concentration of material which will elicit an adverse effect in 50% of the test organisms (i.e., LC50, EC50 or LL50, EL50 for poorly water soluble substances).

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List of species used in aquatic toxic tests

A variety of species are used as standard test organisms in aquatic toxic studies:

Aquatic toxicity tests

Test	Duration	Measurement	Endpoint	Organism	Scientific name	Guideline
Algae	72 hours	Growth, Growth rate	ErC50	green alga	Pseudokirchneriela	OECD 201
			NOEC[5]		Subcapitata	EC.C.3
			NOEC		Scenedesmus	
					subspicatus	
					Chlorella vulgaris[1]	
Acute Invertebrate	48 hours[2]	Immobilisation	EC50	Daphnid (water flea)	Daphnia magna	OECD 202 EC.C.2
Chronic Invertebrate	28 days	Reproduction	EC50 NOEC[5], LOEC[6]	Daphnid (water flea)	Daphnia magna	OECD 202
Acute	96 hours	Mortality	LC50	Rainbow trout	Oncorhynchus mykiss	OECD 203 EC.C.1
Fish				Fathead minnow	Pimephales promelas	
				Bluegill sunfish	Lepomis macrochirus	
				Zebrafish	Brachydanio rerio	
				Common carp	Cyprinus carpio	
				Guppy	Poecilia reticulata	
				Japanese killifish[3]	Oryzias latipes[3]	
				Golden orfe[3]	Leuciscus idus[3]	
Chronic	14 days	Mortality	NOEC	Same as above	Same as above	OECD 204
Fish		Sub-lethal effects	threshold levels			
Chronic						
Fish	28 to 60 days	Hatching, Mortality	NOEC, LOEC	Rainbow trout	Oncorhynchus mykiss	OECD 210
	Post-hatch	Length, Weight		Fathead minnow	Pimephales promelas	
	(dependent upon species)			Zebrafish	Brachydanio rerio	
				Japanese killifish	Oryzias latipes	
				Sheepshead	Cyprinodon variegatus	
				Minnow[4]	Variegatus	

1 Chlorella vulgaris is not described in the EC guideline.
2 EC guideline requires a 48-hour duration.
3 Killifish and Orfe are not listed in the OECD guideline.
4 This is a saltwater species.
5 NOEC (no observable effect concentration).
6 LOEC (lowest observable effect concentration).

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Tests with algae, invertebrates and fish

Tests with algae
Exponentially-growing cultures of selected green algae are exposed to various concentrations of a substance over several generations under defined conditions. Because several generations of algal cells are exposed in this test system, it can sometimes be referred to as a chronic test.

The following endpoints are evaluated:

- Cell density, by microscopic counting of cells or by a spectrophotometric measurement of chlorophyll.
- The inhibition of growth in relation to a control (non-exposed) culture over a fixed period.
- The algal cell density in each flask, at least at 24, 48, and 72 hours after the start of the test. The mean cell density for each concentration is plotted against time to produce growth curves.
- The growth endpoint, by comparing the area under the growth curves for each concentration against the control.
- The average specific growth rate (the increase in cell density over time).

Tests with invertebrates
Acute toxicity tests with invertebrates generally expose organisms to a substance for 48 hours. This period of exposure encompasses at least one sensitive period of growth e.g., during the juvenile life-stage.

In the acute immobilization test with daphnia, effects on the swimming capability of Daphnia magna are investigated. The number of immobile (non-swimming) organisms for each concentration is compared to the control. Immobility is correlated to mortality in these organisms, and it is much more practical to determine if a daphnid is immobile, rather than truly dead(which would require a microscopic assessment of heartbeat).

Tests with fish
A variety of fish are routinely used for acute toxicity tests. One of the most widely utilized species is the rainbow trout, *Oncorhynchus* mykiss.

Fish are exposed to the test substance for a 96-hour period. Mortality observations are performed daily and the median lethal concentration (LC50) is derived for each observation period. The test may be performed under flow-through, semi-static (solution is renewed at regular intervals) or static (no replacement of solution) conditions as long as constant environmental conditions are maintained.

A more recently developed fish embryotoxicity test (FET) exposes eggs of zebrafish to the test substance for a period of 96 hours, after which egg/embryo mortality is observed.

Testing for chronic aquatic toxicity

There are a variety of chronic toxicity test exposures:

- Prolonged toxicity tests (usually two or more weeks).
- Full life cycle test (usually two to three generations).

Measurement of sub-lethal effects
Chronic tests generally evaluate sub-lethal effects, for example:

- Growth (weight or length)
- Development
- Reproduction (fecundity, number of offspring produced)
- Survival of offspring.

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Endpoints

Chronic tests provide more sensitive endpoints than acute EC50 values: NOEC, the No Observed Effect Concentration, and LOEC, the Lowest Observed Effect Concentration, are commonly used. The calculation of LC10/EC10/LL10 for chronic endpoints is increasing in use. These chronic endpoints indicate the concentrations of substance that are (statistically) significantly different from the control.

Tests with invertebrates

A common chronic toxicity test with invertebrates is the Daphnia magna Reproduction Test (OECD 211) in which less than 24-hr old daphnia neonates are exposed to a range of test substance concentrations for 21 days. Within this time, each daphnia will produce several broods, or batches, of young.

This test is performed under semi-static or flow-through conditions. Survival of the parent generation and the number of young produced are evaluated.

Tests with fish

There are two common chronic toxicity tests for fish:

- Early life-stage toxicity test (OECD 210)
- Fish, Prolonged Toxicity Test: 14-Day Study(OECD 204).

Early life-stage test (OECD 210)

It starts with exposure on newly fertilized eggs, through a larger portion of the fish lifespan (this is species-dependent). This test encompasses the embryo, larval, and juvenile stages of various fish species. At termination, all surviving fish are weighed and measured.

NOEC/LOEC values, or LC10/EC10s, are determined based on survival, weight or length, or other abnormal effects observed throughout the test.

A flow-through test design is preferred to semi-static to allow for maintenance of constant water concentrations of the test substance.

This test design allows for evaluation of the following endpoints:

- Mortality during the embryonic stage, larval stage, and juvenile stage
- Days to hatch, and number of organisms hatched
- Length and weight data
- Developmental abnormalities observed.

The exposure period for the early life-stage test varies for each species. For example, tests with warm, saltwater fish can generally be terminated after 28-days post-hatch, whereas tests with cold, freshwater fish (*O. mykiss*) terminate after 60-days post-hatch due to differences in development between species.

Fish, Prolonged Toxicity Test: 14-Day Study (OECD 204)

It is less commonly used. It is performed under similar conditions as the acute toxicity test.
A representative weight and length measurement is taken for the fish, at the start of the test.
The test is performed using either semi-static or flow-through exposure conditions for 14 days.

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Upon entering the environment, a substance may be transported in different ways:

- Within the same environmental medium
- Between environmental media

In addition, the substance may be subjected to a variety of possible transformations. This section presents an overview of how these individual phenomena can be quantified through the combined use of computer modeling and laboratory testing. A brief introduction describing how such information is integrated into modeling frameworks for performing exposure assessments will also be included.

Transport processes

Environmental transport processes can be divided into 2 sorts of movements:

- Movement within a medium: for example, a waste water effluent discharged into a river is transported by the river flow.
- Movement between media: it occurs when a chemical is volatilized from soil into air or is re-suspended from sediment into overlying surface water.

Advection and diffusion

Both types of transfer processes involve advective and diffusive mechanisms. Advection causes the substance to move in the same direction as the media (e.g., air or water currents). Diffusion causes movement in response to concentration gradients (or levels). These transport processes account for the characteristic contaminant plume (or cloud) that is observed down gradient of a point source emission.

Transport can be **within a medium** or **between media** and involve **advective and diffusive mechanisms**

The equilibrium partitioning theory

Environmental media are comprised of different phases. For example, surface water consists not only of an aqueous milieu but also contains suspended solids. Similarly, the atmosphere is comprised not only of air but also particulates referred to as aerosols. An important driving force for diffusive transport is the tendency of a substance to achieve equilibrium between these phases.

Partition coefficients quantify the equilibrium distribution of a substance between different phases:

- The air-water partition coefficient (K_{aw}) is calculated by dividing the HLC by the ideal gas constant (R) and temperature.
- Soil and sediment partition coefficients can be experimentally determined or can be estimated from K_{ow} using empirical QSAR models.
- Gas vapor-aerosol partitioning can likewise be estimated with QSARs that are related to the substance vapor pressure.

The use of equilibrium partitioning theory is an important element of current fate assessments, as the form of the substance influences subsequent transformation and accumulation processes in the environment.

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Examples of important environmental transport processes

Examples of important environmental transport processes

Movement within media	Movement between media
Air advection (winds)	Wet and dry atmospheric deposition
Air diffusion	Volatilisation
Surface water advection (currents)	Gas absorption
Surface water diffusion	Soil leaching/run-off
Surface water advection (currents)	Sediment burial
Surface water diffusion	Sediment-water exchange

Transformation processes: abiotic degradation

To characterize the transformation processes, standardized tests have been defined to allow some prediction of the degradability of chemical substances in the environment. These are generally divided into tests of abiotic degradation (or chemical degradation) and tests of biodegradability.

Abiotic degradation is principally due to photolysis, hydrolysis and oxidation. These reactions convert the chemical into degradation products, but usually do not achieve total conversion to inorganic forms of the constituent atoms (e.g., CO¬, H, H_2O). Thus, an understanding of degradation products as well as the rate is necessary to evaluate environmental effects.

Tests have been standardized for determining the rates of hydrolysis and photolysis.

Photolysis, hydrolysis and **oxidation** reactions convert the chemical into **degradation products**

Hydrolysis

Hydrolysis consists of the decomposition of a substance by water. It is a well understood chemical process. The types of chemicals which hydrolyze and the catalysis of the process have been studied extensively. The standard test for hydrolysis involves preparing aqueous solutions at pH 4, 7 and 9, incubating at 50°C, and analyzing the concentration at various time intervals. Stability for more than a week indicates no significant hydrolysis has occurred. The bonds in hydrocarbons are not hydrolysable under normal environmental conditions.

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Photolysis

Photolysis depends upon the absorption of sunlight with a wavelength greater than 290 nm. Sunlight intensities are too low at shorter wavelengths to cause photolysis. Molecules need to have a strong adsorption band in this region to undergo significant photolysis in the environment, so the UV/Visible spectrum of chemicals is used to screen for the likelihood of photolysis. Photolysis is an unlikely fate pathway for ExxonMobil Chemical fluids or to Jayflex™ plasticizers, Exxal™ alcohols and ExxonMobil™ neo acids.

Photooxidation

Atmospheric photo-oxidation is the degradation of chemicals in air due to reaction with ozone or hydroxyl radicals. Hydroxyl radical attack is the predominant mechanism for most chemicals. Hydroxyl radicals are produced through the interaction of sunlight with oxygen and other substances in the atmosphere. The reaction is dependent upon the structure of the chemical, its concentration, and the hydroxyl radical concentration. Due to their volatility, hydrocarbon solvents are rapidly oxidized in air through hydroxyl radical attack.This is the main environmental fate for most hydrocarbons.

There is a considerable amount of test data on the rate of hydroxyl radical reaction for chemicals, and this has allowed the development of QSAR models for calculation of atmospheric half-lives.

Transformation process: biodegradation

Bioaccumulation processes

Bioaccumulation processes result in the direct or indirect transfer of a substance from primary environmental media (i.e., air, water, soil, sediment) to secondary media (i.e., aquatic and terrestrial plants and animals).

Substances which typically pose the greatest concern for bioaccumulation potential, such as certain chlorinated insecticides (e.g., DDT) and polychlorinated biphenyls (PCBs), have the following characteristics:

- Use of diffuse sources (e.g., pesticide application) to enter the environment
- Poor degradation in primary media
- A high lipophilicity
- Resistance to biochemical transformation (metabolic breakdown) by plants and animals.

Different tests are used to assess bioaccumulation:

Lab and field tests: BCF and BAF

The bioconcentration factor (BCF) and the bioaccumulation factor (BAF) are commonly used to quantify bioaccumulation potential by aquatic organisms. The units of both BCF and BAF are L/kg wet weight (i.e., mg/kg wet weight ÷ mg/L).

BCF: a lab measurement

The BCF is a lab measurement that reflects accumulation due only to aqueous exposure in the laboratory. BCF measurements are applicable to test substances that are well-defined single components rather than complex mixtures.

BAF: a field measurement

The BAF is a field-derived measurement determined from monitoring data. It is calculated by dividing the observed field tissue concentration by the corresponding dissolved concentration in water. It reflects accumulation via all possible exposure routes that may occur in the field (i.e., water, sediment, diet).

Although BAFs provide a more realistic appraisal of field bioaccumulation, they exhibit a high degree of uncertainty due to the variability of the environment and associated contaminants. Moreover, reliable field datasets for computing BAFs are often not available. Consequently, BCF provides a valuable surrogate parameter for assessing the relative bioaccumulation potential of different substances under controlled laboratory conditions.

A wide range of global regulatory bioaccumulation criteria exist. Some regulators consider that substances with a BCF above a defined value are a risk for bioaccumulation. Others, in the absence of BCF data, use K_{ow} values to assess bioaccumulation potential.

Assessment models have evolved from the early QSARs and are now considered more realistic because they incorporate the impact of biotransformation on bioaccumulation into the prediction of BCFs. Dietary bioaccumulation experiments demonstrate how biotransformation limits the bioaccumulation potential of petrochemicals.

OECD 305 test
The OECD 305 test is used to characterize the bioconcentration potential of substances in fish. It consists of both uptake and depuration phases from which a simple model is derived to estimate the BCF and the half-life for the test substance.

During the uptake phase, aquatic organisms are exposed to a constant aqueous exposure concentration of the test substance. At periodic intervals, organisms are sampled and analyzed to determine tissue concentrations.

Once steady state tissue concentrations are approached, the test organisms are transferred to clean water to determine how rapidly the test substance is lost from tissues. Based on the measured tissue concentrations obtained during uptake and depuration periods, a simple model is generally used to estimate the BCF and the half-life for the test substance.

Dietary exposure and test method
A dietary exposure test is similar in design to a BCF test except organisms are exposed to the substance via food rather than water. Test results are expressed in terms of a biomagnification factor (BMF) which represents the steady-state concentration in the organism to that in its diet both expressed on a lipid-normalized basis:

- If the BMF > 1, the substance is expected to undergo biomagnification.
- If the BMF is near unity, bioaccumulation is described by simple equilibrium partitioning.
- If the BMF < 1, the substance is expected to undergo biodilution, and concentrations decrease in higher trophic levels (e.g., daphnia are consumed by fish; with biodilution, the fish will have a lower concentration of the test substance than the daphnia).

QSARs for bioaccumulation potential in the terrestrial food chain
Standardized laboratory testing procedures to assess bioaccumulation potential in the terrestrial food chain are generally lacking. Limited data from laboratory experiments and field monitoring studies have been used to develop empirical QSARs for estimating bioaccumulation potential in the terrestrial food chain.

For example, QSARs are available for estimating the transfer of contaminants from air and soil to plants and from plants to beef and milk. However, these QSARs are based on data for a few substances from a limited number of chemical classes (e.g., chlorinated organic compounds). Consequently, the general applicability of such QSARs to other industrial chemical classes is highly uncertain and likely to be very conservative since the influence of biotransformation is usually ignored.

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Fate models

The relative importance of the various fate processes may be quantitatively evaluated through the use of mathematical models that are translated into computer algorithms. Environmental fate models can be broadly grouped into two categories:

Site-specific models

Examples include atmospheric dispersion or effluent dilution models. The purpose of these models is to characterize the environmental fate and exposure in the vicinity of a point source release.

Generic evaluative models

Generic evaluative models provide a broader understanding of the key fate processes and multimedia distribution of a substance at the regional or continental scale. As a result, typical properties of the environment are assumed (e.g., volumes of air, water, soil, sediment, wind speed, rainfall, etc.). Depending on complexity, evaluative models can be further categorized into three levels.

Generic evaluative level I models

A Level I model assumes simple equilibrium partitioning between environmental compartments (e.g., air, water, soil, sediment) based only on the physicochemical properties of the substance. Since degradation processes are ignored, the Level I model provides the least realistic assessment of environmental exposure.

Nevertheless, Level I models provide useful insights regarding which environmental compartment(s) has the greatest influence on the environmental behavior of a substance and supports the distinction between environmental classification and the actual risk of that substance.

These insights are important in highlighting the distinction between environmental classification and the actual risk posed by such substances. For example, several Isopar™ products exhibit aquatic toxicity when tested in closed laboratory systems with no headspace (i.e., no air space in the test system for the substance to evaporate to). However, in reality these substances are not expected to present a high environmental risk, because physical properties like volatility, limit the actual (aquatic) environmental exposure potential, since there would be a high amount of volatilization in a real-world scenario.

Generic evaluative level II and III models

A Level II model is based on simple equilibrium partitioning but includes consideration of biotic and abiotic degradation processes in each environmental compartment.

A Level III model does not assume equilibrium partitioning and considers limitations in mass transfer between compartments. Therefore, unlike Level II, the results of a Level III model depend upon, not only the total amount emitted, but also the emission scenario, i.e., the compartment(s) to which the substance is released.

Assess environmental persistence

Level II and III evaluative models are increasingly being used in various regulatory initiatives to assess the environmental persistence and long range transport of substances:

- Persistence is a measure of the environmental lifetime of a substance
- Long range transport potential indicates how far a substance travels during its lifetime in the environment.

Environmental exposure assessment

The objective of an environmental exposure assessment is to provide a quantitative and qualitative estimate of the substance dose or concentration to which the population and the environment may be exposed. It may consider all stages of a substance's life cycle – production, uses and waste - in order to estimate the amount of emissions released and environmental concentrations.

EU REACH initiated the development of exposure assessment and it enforces a strict process for substances to be evaluated on the basis of hazard and risk throughout the supply chain. Since then TSCA in the US has also evolved in that direction.

Key concepts »

The key concepts of environmental exposure assessment are the geographic scale and the end-points of exposure estimation: PECs and PNECs

Release estimation: ERCs and SpERCs »

Release estimation is the process whereby releases to the environment are quantified during the life cycle stages of a chemical.

Exposure estimation »

Exposure estimation is a critical step in the exposure assessment process and consists in determining operational conditions and risk management measures.

Downstream users obligations »

REACH has set up a strict process whereby exposure scenarios are attached to the safety data sheets and communicated down the supply chain.

Further guidance on exposure assessment »

Further guidance on how to develop an exposure assessment is available here.

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Key concepts

The key concepts of environmental exposure assessment are:

- The geographic scale
- The end points of exposure estimation: PECs and PNECs

Local and regional scales

The exposure to the environment is in principle assessed on two spatial scales:

- Locally, in the vicinity of point sources of release to the environment, for example in the air, in local grassland, fields or water
- Regionally for a larger area which includes all point sources and wide dispersive sources in that area.

Releases at the continental scale are considered to provide inflow concentrations for the regional environment.

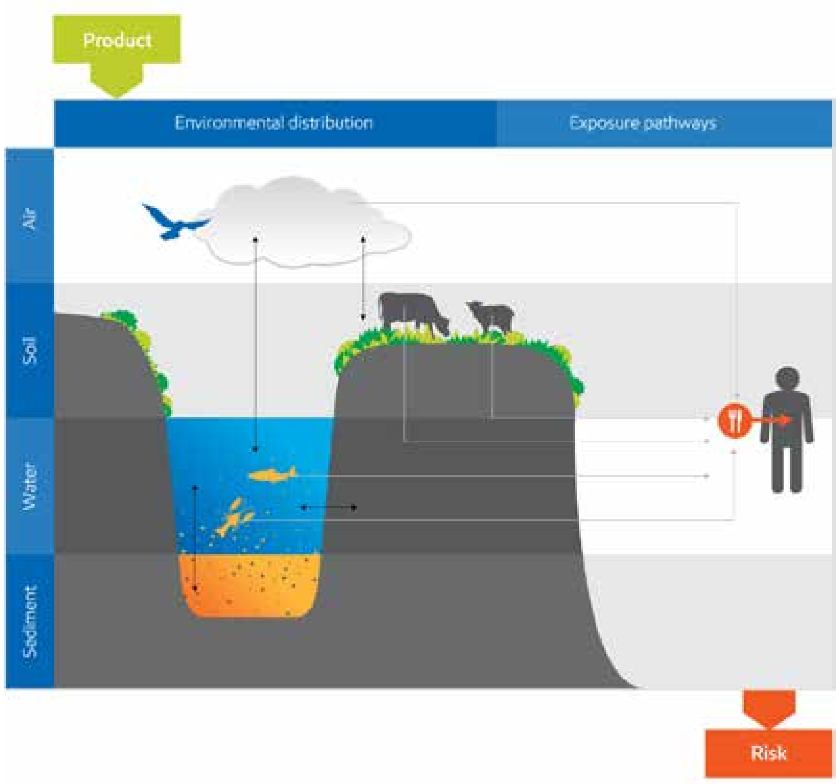
The end points of exposure estimation: PECs and PNECs

The end results of the exposure estimation are **predicted environmental concentrations (PECs)** in environmental compartments such as air, surface water (fresh and marine), soil, sediment, and biota (e.g., earthworms and fishes for secondary poisoning), as well as human daily intake of the substance via the environment for both local and regional scale.

PECs are a result of both:

- Releases of the chemical into the environment for the development of exposure scenarios
- Fate processes taking place after release, resulting in chemical distribution to various environmental compartments (air, soil, water, sediment, biota) at certain concentration levels and including passive transport with water and air (i.e., advective exchange between compartments), diffusion, degradation or sedimentation.

The risk assessment process then compares the PECs to the substance concentration at which no harmful effect on the environment is expected, or the predicted no effect concentration (PNEC). In this respect, it is critical that the risk assessment incorporates emissions from different sources into the same compartment, so that cumulative exposure is also evaluated.



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Release estimation: ERCs and SpERCs

Release estimation is the process whereby releases to the environment are quantified during the life cycle stages of a chemical.

The information that needs to be considered for the release estimation is:

- Tonnage of substance used or produced
- Life cycle stage
- Type of use in the life cycle stage
- Distribution of production volume in the market
- Emission pattern – distribution in time and special scale
- Emission pathways (air, soil, water)
- Multiple emissions
- Emission factors
- Receiving environmental compartments
- Risks management measures (RMM) to reduce emissions

For each environmental compartment (air, soil, water, sediment) potentially exposed, the exposure concentrations, or predicted environmental concentrations (PECs), are derived either by **measurement (monitoring data)** or by **model prediction**, taking into consideration distribution and fate processes after the chemical has entered the environment.

ERCs and SpERCs have been developed to streamline the **release estimation and data collection**

Relevant measured data from substances with analogous use and exposure patterns or analogous properties, if available, are also considered when applying model calculations.

To streamline the release estimation and make it accessible for data collection in the supply chain, environmental release classes (ERCs) and specific environmental release classes (SpERCs) have been developed and mapped. Both are required for:

- Predicting relevant emissions to the environment linked to occupational activities and article categories
- Grouping substance uses from an environmental perspective
- Carrying out initial exposure estimates taking risk management measures into account
- Communicating on emissions and releases in the supply chain
- Providing input parameters (together with product tonnage and risk management measures) that are needed to calculate releases during the life-cycle of a substance.

Environmental release classes (ERCs)

Environmental release classes (ERCs) describe representative use patterns of substances and give a first indication of the potential of a substance to be released to the environment. They have been mapped to each generic exposure scenario (GES) title.

Each ERC is linked to fixed, default environmental release fractions that can be used to estimate release rates to the relevant environmental compartments (air, water, soil). These release fractions are, however, highly conservative and often require refinement for exposure assessment.

More realistic parameter values associated with operational conditions (OCs) (e.g., site tonnage, release fractions, etc.) and risk management measures (RMM) are provided by specific environmental release categories (SpERCs).

For more information:

- ECHA guidance on the use descriptor system
- ECHA guidance on information requirements and chemical safety assessment chapters - R.12: use descriptor system
- ECHA guidance on information requirements and chemical safety assessment R.16: environmental exposure estimation

Specific environmental release classes (SpERCs)

SpERCs have been developed by the industry to comply with the REACH requirements for environmental release classes (ERCs), but with realistic data and assumption for a particular use (e.g., site tonnage, release fractions, etc.) instead of using the default conservative set of exposure conditions.

While SpERC parameter values are generic, they have been derived from literature values and/or industry knowledge and are typically much less conservative than the values associated with ERCs.

The SpERCs developed by ESIG/ESVOC have been entered in the ECETOC TRA exposure tool for assessing single substances and the Petrorisk model for assessing complex mixtures.

The CHESAR (CHEmical Safety Assessment and Reporting) tool is the latest tool, developed by the European Chemicals Agency (ECHA), also capable of utilizing pre-defined SpERC determinant files. If the results from an assessment using environmental release categories (ERCs) suggest the need for reasonable risk management measures, it is not necessary to perform the same assessment using SpERCs. It is at the assessor's discretion to choose to move from ERCs to SpERCs or start from the beginning using SpERCs. It is also important for the assessor to recognize and understand the boundary conditions/limitations of each SpERC.

Exposure estimation

In order to comply with the EU REACH legislation, exposure estimation is a critical step in the whole process of environmental exposure assessment.

It consists in determining **operational conditions (OCs) and risk management measures (RMMs)**, including, for example:

- Amount of substance;
- Process temperature;
- Duration and frequency of use or activity;
- Industrial wastewater treatment plants, filters, scrubbers;
- Municipal sewage treatment plants etc.

Its ultimate purpose is to compare the **predicted environmental concentration (PEC)** for environmental compartments of interest, i.e., water, sediment, soil, air and top-predators to the **predicted no effect concentration (PNEC)**, which is required to assess risk **and calculate the risk characterization ratio (RCR)**.

Generic exposure scenarios (GES) and scaling solutions

Generic exposure scenarios (GESs) represent an efficient and pragmatic solution for evaluating and communicating health and environmental risks. They identify:

- How a substance is used and how it is handled.
- What operational conditions (OCs) are typical of each of its life-cycle steps.
- What risk management measures (RMMs) are enforced.
- What potential exposures can affect the environment and workers.

Each GES contains several contributing scenarios – or default scenarios - which describe the handling activities of the substance within one life cycle step, i.e., a specific use of the substance. A substance exposure scenario (ES) describes the typical conditions under which the use of a specific substance within one life cycle step is considered safe. All these factors, along with specific predicted no effects concentration (PNEC) for environment and derived no effect level (DNEL) for human health of the substances, are required to assess risk and to calculate the risk characterization ratio (RCR).

For the environment, typical OCs are defined within a specific environmental release category (SpERC) and can be used for the chemical safety assessment (CSA) when documented in a factsheet. In some instances, the typical OCs defined will not lead to safe use, e.g., for highly toxic substances used in very high volumes. In such cases, registrants will need to modify the GES data and additional RMMs may be required to ensure safe use, e.g., personal protection equipment.

Once the conditions for safe use have been established, the exposure scenarios are documented in a chemical safety report (CSR) and communicated down the supply chain by annexing them to the safety data sheet (SDS) to make the extended safety data sheet (ext-SDS), as required by REACH. ExxonMobil Chemical has been at the forefront of industry efforts in this area, working closely with groups such as ESIG (ESIG on GES). As a result, our extended safety datasheets (ext-SDSs) fully incorporate the GES principles and solutions. Widely endorsed, GESs have been incorporated into the European Chemicals Agency (ECHA)'s chemical safety assessment and reporting tool (Chesar) and the CEFIC guidance on REACH exposure scenarios.

Scaling solutions
When conditions of use slightly fall outside the frame defined by the GES, there is a solution: scaling, an activity that must be carried out by the user of the substance. It is intended to determine if the exposure controls identified in the exposure scenarios (ESs) contained in ext-SDS are consistent with those being applied by the user. It identifies what actions are necessary if either the use has not been registered or local exposure control conditions differ significantly to those outlined in the GES.

We can help you define scaling solutions if your conditions are outside the GES frame

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If you would like more information on scaling techniques and solutions, please contact your sales representatives.

Risk characterization and the Petrorisk model

In order to characterize the risk of an exposure scenario in which emission to the environment occurs, the predicted environmental concentration (PEC) is compared to the safe limit value for the environmental compartment of interest (PNEC) to calculate the risk characterization ratio (RCR) for each environmental compartment.

Risk characterization ratio (RCR)
The equation for calculating the **RCR is**: $\mathbf{RCR}_{\text{ENVIRONMENT}}$ **= PEC / PNEC**, where PNEC is the highest concentration that has no effects on the environment. PNECs can be different values for the different environmental compartments:

- Aqueous environment (freshwater and marine water)
- Sediment (freshwater and marine water)
- Terrestrial environment
- Secondary poisoning, i.e., effects that can appear as a result of accumulation in the food chain.
- Possible effects on the microbial activity in sewage treatment

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Estimating the **risk of substance emission** in **various environmental media** is critical

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The Petrorisk model
Petrorisk is a spreadsheet tool that performs environmental risk assessments for petroleum substances using principles provided by the European Chemical Agency (ECHA) for fulfilling stakeholder obligations under the EU REACH regulation. It is based on the ECHA REACH implementation guidelines for performing risk assessments of complex petroleum substances using the hydrocarbon block method.

The Petrorisk model can evaluate risks associated with different stages in the product life cycle at local and regional scales, e.g., at the production, formulation, and distribution stages as well as for generic uses in industrial, professional and consumer use sectors.

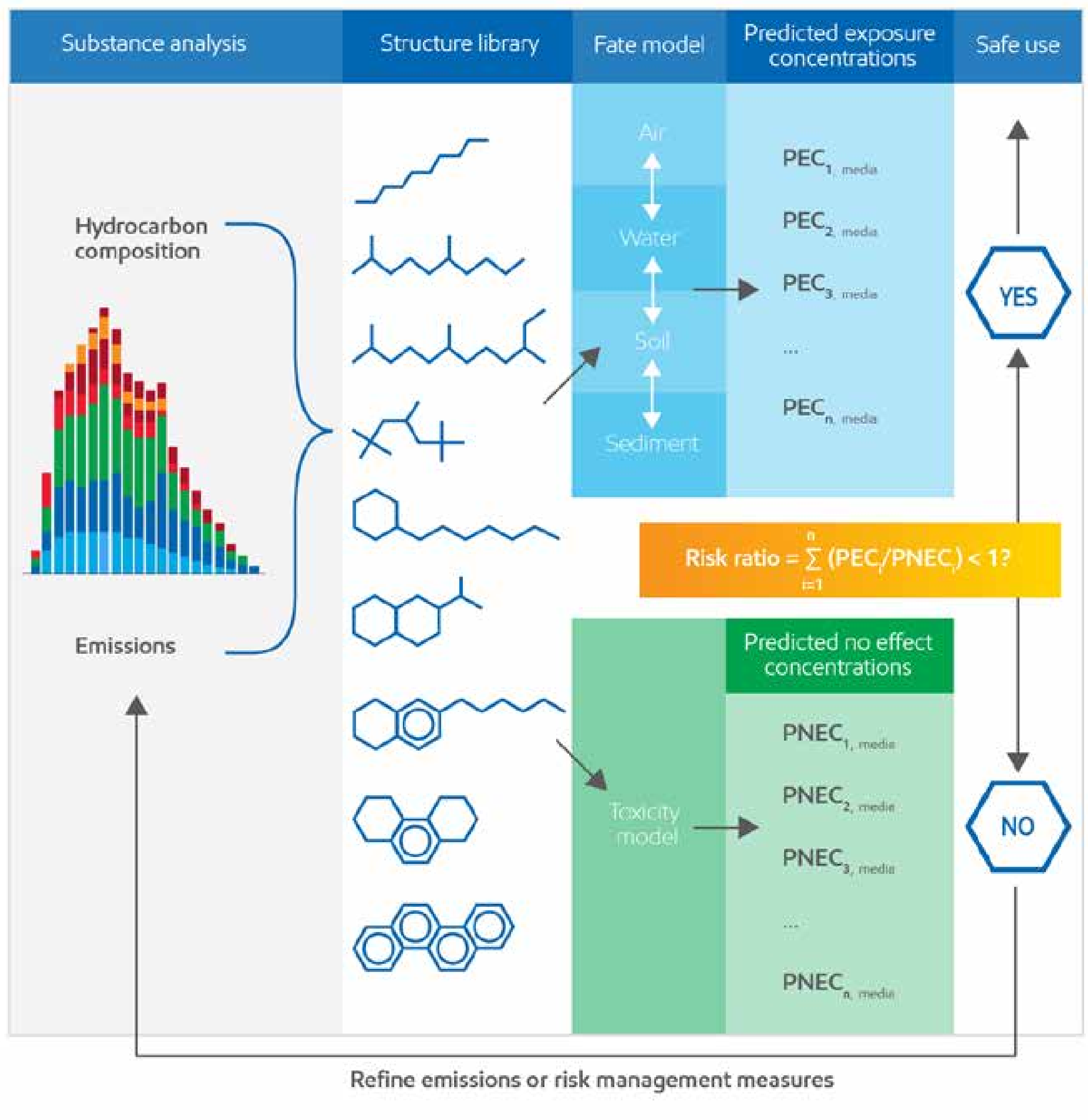
It calculates the predicted environmental concentrations (PECs) of representative hydrocarbons assigned within blocks (defined by compositional analysis) in various compartments of soil, air, water, waste water treatment plant (WWTP) effluent, drinking water, fish, meat and milk based on results obtained from the EUSES multimedia exposure model.

For water, effluent, soil and sediment compartments, PECs are divided by predicted no effect concentrations (PNECs) to compute environmental risk quotients (RCRs):

- Ecological risks for these compartments are then quantified by adding the PEC/PNEC ratios for the representative hydrocarbon structures that are used to simulate the hydrocarbon blocks comprising the substance. A risk quotient of ≥1 indicates a potential unsafe use.
- Human exposures are also calculated for total hydrocarbons using a default set of exposure pathways specified by EUSES. User-defined derived no effect levels (DNELs) that are expressed in terms of total hydrocarbon exposure or dose can be entered to perform human health risk assessment.

A schematic of the exposure and risk assessment calculations for hydrocarbon UVCBs (unidentified and variable composition and biological) using the Petrorisk model:

Environment – Environmental exposure assessment – Risk characterization



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Downstream users obligations

Europe was the first region to apply risk assessment following a standardized process as part of EU REACH. The United States are exploring a similar route but nothing is defined yet.

According to EU REACH, the exposure scenarios (ES) are communicated down the supply chain by annexing them to the safety data sheet (SDS), i.e., the extended safety data sheet (ext-SDS).

Downstream users (DUs) must pass on exposure scenarios further down the supply chain where relevant. DUs have to verify whether the exposure scenarios that are received via an ext-SDS describe the conditions for their applicable uses on-site.

- First, a check needs to be done to see if the identified uses of a DU are included via the ES titles, use descriptors, main exposure determinants.
- Then, a check to see if all recommended operational conditions (OCs) and risk management measures (RMMs) are in place.

If DUs are in compliance with the conditions in the relevant ESs, this needs to be documented and they must be able to show this information to the authorities in case of inspections.

Exposure assessment is the responsibility of manufacturers and **downstream users**

If not, several options are available:

- Implementation of the recommended RMMs and OCs
- Communication to the supplier of the on-site conditions the DU has in place, with a request to update the relevant ES accordingly
- Preparation of a DU chemical safety assessment
- Scaling: recalculate exposure & risk using modeling tools using the on-site conditions.

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Further guidance on exposure assessment

The European Chemicals Agency (ECHA) has developed documents to provide guidance on exposure assessment:

- ECHA guidance on information requirements and chemical safety assessment chapters - R.12: use descriptor system
- ECHA guidance on information requirements and chemical safety assessment R.16: environmental exposure estimation

Please visualize an example of an exposure assessment in the annex of a safety data sheet.

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VOCs and outdoor air quality

Volatile organic compounds (VOCs) are chemical substances that can evaporate under normal atmospheric conditions. On a global basis, the major source of VOCs is from natural emissions (e.g., from pine trees or agriculture) or transport fuel, with a small portion coming from solvents.

VOCs have minimal direct impact on the environment. It is their interaction with other factors in the atmosphere that may affect the environment.

Although solvents cover a wide variety of substances, our VOC focus will be on oxygenated and hydrocarbon solvents, the only solvents produced by ExxonMobil Chemical. Jayflex™ plasticizers, Exxal™ alcohols and ExxonMobil™ neo acids are not very volatile by nature and generally not used as solvents.

Key concepts »

The reactions between VOCs and other substances present in the atmosphere that can result in the formation of ozone and particulate matter (PM) and determine the impact of VOCs on the environment.

Effects of VOCs in the atmosphere »

The 3 main air quality issues to consider are: tropospheric (ground level) ozone, particulate matter and climate change.

Atmospheric reactivity »

Depending upon their chemical structure, VOCs differ in their potential to participate in atmospheric reactions leading to ozone formation.

VOC emission management »

Controlling the emissions of VOCs requires a systematic approach: an inventory of all emission sources, quantification of the amounts emitted as well as an emission reduction plan.

VOC and outdoor air quality regulations »

Here is an overview of the main regulations concerning VOCs – in Europe and in the US.

Key concepts

The main elements that should be considered and understood when assessing the impact of oxygenated and hydrocarbon solvents on the environment are: VOCs, ozone and particulate matter.
The reactions between VOCs and other substances present in the atmosphere that can result in the formation of ozone and particulate matter (PM) determine the impact of VOCs on the environment.

VOCs

A few definitions are necessary to help us understand how VOCs impact the quality of the air: organic compound, volatile organic compound (VOC) and vapor pressure, the main measure. They help clarify the differences associated with various regulatory definitions across the globe.

Organic compound

An organic compound contains at least the element carbon and one or more of hydrogen, halogens (e.g., chlorine, fluorine or bromine), oxygen, sulphur, phosphorus, silicon, or nitrogen. The exceptions to this definition are carbon oxides and inorganic carbonates and bicarbonates.

Defining **organic compound, VOC and vapor pressure** helps clarify **regulatory differences** across the globe

Volatile Organic Compound (VOC)

Volatile organic compounds (VOCs) are organic chemical substances that can evaporate under normal atmospheric conditions. On a global basis, the major source of VOCs is from natural emissions (e.g., from pine trees or agriculture) or transport fuel, with a small proportion coming from solvents. The definition of Volatile organic compounds (VOCs) varies depending on the regulatory use and the region. Their definition is either based on boiling point or volatility limits, or participation in atmospheric chemical reactions.

Examples include:

In Europe:

- EC Directive 1999/13/EC (Solvent Emissions Directive):
- The most commonly used VOC definition in EU for solvents is: organic compounds having at 293.15 K (i.e., 20°C) a vapor pressure of 0.01 kPa or more, or having a corresponding volatility under particular conditions of use.
- Paint Directive 2004/42/EC:
- Organic compounds having an initial boiling point lower than or equal to 250 °C at an atmospheric pressure of 101.3 kPa.
- EU National Emissions Ceilings Directive 2001/81/EC:
- any organic compound of anthropogenic nature, other than methane, that is capable of producing photochemical oxidants by reaction with nitrogen oxides in the presence of sunlight.

In the US:

- VOCs are any organic compound which participates in atmospheric photochemical reactions. Organic compounds which have been determined to have negligible photochemical reactivity (lower than ethane) are excluded from the definition.
- A Low Vapor Pressure (LVP) exemption exists for consumer products. VOCs with a vapor pressure lower than 0.1 mm Hg at 20oC are not included in the weight-percent VOC calculation for the product (Federal Register 1998 - Vol 63 No 176).

Vapor pressure
The volatility of VOCs is defined by evaluating their vapor pressure:

- Volatility is the tendency of a solid or liquid material to pass into the vapor state at a given temperature (Hawley's Condensed Chemical Dictionary).
- Vapor pressure is the pressure characteristic at any given temperature of a vapor in equilibrium with its solid and liquid phase (Hawley's Condensed Chemical Dictionary). The vapor pressure of pure chemical substances is generally well known.

The ESIG vapor pressure tool: an industry standard to help assess whether hydrocarbon solvents are VOCs

The European Solvent Industry Group (ESIG) has developed a tool to estimate the vapor pressure of complex hydrocarbon solvents of low volatility (with vapor pressure around 0.01KPa at 20°C) and to evaluate the products against the VOC definition according to the Directive 2010/75/EU on industrial emissions.
Adopted as an industry standard, the tool is available on the ESIG website.

For more information, please contact your ExxonMobil sales representative.

Ozone

It is important to understand how VOCs react in the different ozone layers. Ozone (O3) is a very reactive form of oxygen and a powerful oxidant. It is a gas that is found in the stratosphere and the troposphere:

- **Stratosphere** (more than 10 km above the ground): stratospheric ozone is beneficial to human health and the environment because it absorbs the aggressive ultraviolet (UV) rays and protects us from their adverse effects.
- **Troposphere** (the lowest layer of the atmosphere, from sea level to 10-16 km above the ground): ozone at ground level serves no known protective or beneficial role, but has been shown to be a clear hazard to the human respiratory tract

Oxygenated and hydrocarbon solvents belong to the category of VOCs that have no impact on stratospheric ozone. However, under certain conditions they may react in the troposphere and contribute to the formation of tropospheric ozone.

How is ozone produced?

$$NO_2 + h\nu\ (\text{UV light}) \rightarrow O^{\cdot} + NO^{\cdot}$$
$$O^{\cdot} + O_2 \rightarrow O_3$$
$$O_3 + NO^{\cdot} \rightarrow NO_2 + O_2$$

The creation of ground-level ozone is a complex process. In order to occur, the interaction of 3 elements is required:

1. Nitrogen oxides (NOx). Highly polluting gases produced from combustion, e.g., in an engine, and causing smog and acid rain
2. Volatile organic compounds (VOCs) (e.g., unsaturated hydrocarbons)
3. Sunlight

Without NOx and sunlight, VOCs cannot create ground-level ozone. At night time, no ozone can be formed. In the presence of NOx, VOC radicals interact with the nitrogen oxides radicals and this leads to the formation of ground-level ozone.

VOCs from different chemical species have different potential for creating ground-level ozone.

Particulate matter

VOCs interact with atmospheric particulate matter (PM or particles) and it is therefore important to distinguish between primary and secondary PM:

- **Primary PM** is made of particulate emissions composed mostly of crustal dust (particles originating from the earth's crust) and organic and elemental carbon particles
- **Secondary PM** is particulate matter formed via atmospheric reactions of gaseous emissions and falls into two categories:
  - *secondary inorganic aerosols*, that is ammonium nitrates, ammonium sulfates and ammonium and chloride aerosols
  - *secondary organic aerosols* (SOAs), formed from organic compounds via photochemical reaction.

Solvent VOCs are a **minor contributor** to total particulate matter.

Secondary Organic Aerosols (SOAs) are formed in the atmosphere by the condensation of low vapor pressure products of the oxidation of organic gases. They can be formed by three processes: chemical reactions of gaseous compounds to yield a product at a concentration greater than its atmospheric saturation concentration; condensation on solid surfaces (adsorption); and condensation on liquid droplets (absorption).

Chemical structures that favor SOA formation include double bonds, aromatic rings and molecular weights between C6 and C10. Chemical characteristics of some natural VOCs, such as monoterpenes, favor aerosol formation.

Particulate matter is important because it travels in the air and we all breathe it. Solvent VOCs are a minor contributor to total PM. They can participate in atmospheric reactions leading to secondary organic aerosol (SOA) formation.

Effects of VOCs in the atmosphere

Currently, there are 3 main air quality issues related to emissions of oxygenated and hydrocarbon solvent VOCs in the atmosphere:

- Tropospheric (ground level) ozone
- Particulate matter
- Climate change

VOCs and ozone

Ozone is a powerful oxidant. At high concentrations, it can be harmful to humans and cause damage to the environment.
Regulatory air quality standards therefore exist to limit ground level ozone and avoid pollution peaks. International regulations are being developed to decrease emissions of nitrogen oxides (NOx – which are also required to be present for the ozone creating reaction to occur) and VOCs.

Effects of ozone on human health

Under certain conditions, ozone levels in the troposphere may exceed maximum values set by the World Health Organization: 100 µg/m3 or 50 ppb as a maximum daily 8-hour average. High levels of O3 in the troposphere have been linked to human health effects, such as irritation of the eyes and respiratory tract, which can produce coughs and chest congestion, and respiratory ailments. People with existing respiratory disease (such as asthma and bronchitis) are believed to be most susceptible to the effects of ozone.

Effects of ozone on vegetation

Ozone can enter plant leaves through the stomata (surface pores through which air enters the plant), penetrate the cell wall and damage the cell membrane, and other cell structures. By damaging parts of the plant cell, ozone can inhibit photosynthesis, reduce movement of sugars from the shoots to the roots and hasten the process of leaf aging and loss. Lesions in the plant tissue and lower crop yields may result from overexposure to ozone.

For more on VOCs and ozone modeling (from ESIG, the European Solvents Industry Group), click here.

VOCs and particulate matter

The size of particles is important. Smaller particle sizes can enter human airways and bloodstream.

Solvent VOCs are a minor contributor to total particulate matter (PM) and they may participate in atmospheric reactions leading to secondary organic aerosol (SOA) formation. Because PM can affect human health, air quality standards exist to limit PM.

VOC contribution to SOA formation **from natural sources is 10 times greater** than from man-made VOCs.

Recent studies indicate that VOC contribution to SOA formation from natural sources is 10 times greater than the contribution from man-made VOCs. Of man-made VOCs, the most important contributors to PM are aromatic compounds. However, the overall contribution of aromatic compounds to SOA is considered minor. The photo-oxidation of aromatic compounds is estimated to represent 10% of the total SOA yield from natural and man-made hydrocarbon emissions.

In this global picture, the contribution of solvents to the formation of SOAs is very small.

VOCs and climate change

Solvent VOCs can form CO_2, O_3 and secondary organic aerosol (SOA) but are estimated to have a minimal effect on climate change compared to other sources.

It is generally accepted that the presence of increased levels of "greenhouse gases" in the atmosphere may have an effect on global climate, although this process is quite complex. By allowing incoming solar radiation to penetrate the earth's surface and re-absorb infrared radiation emanating from it, greenhouse gases can promote the heating of the earth's surface.

Carbon dioxide and methane, and to a lesser extent N_2O and chlorofluorocarbons, are the primary greenhouse gases. Ozone in the upper troposphere is a minor greenhouse gas.
VOCs are not greenhouse gases and are therefore not directly implicated in global warming. However, degradation and burning of VOCs result in the formation of carbon dioxide and possibly ozone. As such, VOCs are indirectly implicated in the global warming process, although they can also participate in atmospheric reactions leading to SOA formation with a cooling effect.

The contribution of solvents to carbon dioxide (CO_2) emissions is generally accepted as negligible in comparison with other sources.

To learn more about this topic, please click here (ESIG, the European Solvents Industry Group).

Atmospheric reactivity

Depending upon their chemical structure, VOCs differ in their potential to participate in atmospheric reactions leading to ozone formation. Several different metrics are used to express the relative potential of a VOC to participate in atmospheric chemical reactions leading to ozone formation. The process can be called atmospheric reactivity or VOC reactivity or photochemical reactivity.

The two most common metrics are:

- Photochemical ozone creation potential (POCP) commonly used in Europe
- Maximum incremental reactivity (MIR) commonly used in the US

POCP

The POCP scale represents a continuum of chemical reactivity potentially leading to formation of tropospheric ozone. The calculation of POCP requires the estimation of VOC and NOx emissions and modeling the transport of the air while considering the many reactions occurring among the constituents in the troposphere.

Because meteorology and emissions vary for different locations, POCP estimates of specific hydrocarbons will differ between geographical regions. However, the relative ranking of individual chemicals will not change appreciably given similar assumptions. The assumptions of Derwent's analyses are designed to yield POCP estimates representative of the relative contribution to ozone formation on a regional basis. Relative rankings of POCP values calculated using other assumptions, such as shorter time scales, showed greater variation; shorter time scales may be more representative of local rather than regional analyses.

POCP values for selected organic compounds

POCP values for selected organic compounds determined for European multi-day conditions from (1) Derwent et al., 2007 and (2) MIR values in US CARB from Carter 2010.

Alkanes

VOC species	POCP[1]	MIR[2]
Ethane	8	0.28
Propane	14	0.49
Butane	31	1.15
i-Butane	28	1.23
Pentane	40	1.31
i-Pentane	34	1.45
Neopentane	18	0.67
Hexane	40	1.24
2-Methylpentane	41	1.5
3-Methylpentane	43	1.8
2,2-Dimethylbutane	22	1.17
2,3-Dimethylbutane	50	0.97
Heptane	35	1.07
2-Methylhexane	32	1.19
3-Methylhexane	42	1.61
Octane	34	0.9
2-Methylheptane	34	1.07
3-Methylheptane	37	1.24
Nonane	34	0.78
2-Methyloctane	34	0.83
3-Methyloctane	34	0.99

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Alkanes (cont.)

VOC species	POCP[1]	MIR[2]
4-Methyloctane	37	0.95
3,4-Dimethylheptane	36	1.24
Decane	36	0.68
2-Methylnonane	35	0.73
3-Methylnonane	39	0.75
4-Methylnonane	35	0.86
2,5-Dimethyloctane	38	1.03
2,6-Dimethyloctane	36	1.08
2-Methyl-3-ethylheptane	34	0.99
2,2-Dimethyl-3,3-dimethylhexane	19	
Undecane	36	0.61
2-Methyldecane	34	NA
3-Methyldecane	36	0.65
4-Methyldecane	36	0.68
5-Methyldecane	35	NA
Dodecane	33	0.55
Tridecane	42	0.53
Tetradecane	46	0.51

Cycloalkanes

VOC species	POCP[1]	MIR[2]
Methylcyclopentane	49	2.19
Cyclohexane	28	1.25
Methylcyclohexane	65	1.7
Ethylcyclohexane	63	1.47
Propylcyclohexane	60	1.29
1,2,3-Trimethylcyclohexane	57	1.22
i-Propylcyclohexane	60	1.29
Butylcyclohexane	59	0.99
i-Butylcyclohexane	59	0.99
1-Methyl-3-propylcyclohexane	60	NA
1-Methyl-4-propylcyclohexane	56	NA
Pentylcyclohexane	56	0.84
Hexylcyclohexane	56	0.65

Alkenes

VOC species	POCP[1]	MIR[2]
Ethylene	100	9.0
Propylene	117	11.66
But-1-ene	104	9.73
Cis-but-2-ene	113	14.24
Trans-but-2-ene	116	15.16
Butylene	63	NA
1,3-Butadiene	89	12.61
Cis-pent-2-ene	109	10.38

Alkenes

VOC species	POCP[1]	MIR[2]
Trans-pent-2-ene	111	10.56
1-Pentene	95	7.21
2-Methylbut-1-ene	75	6.4
3-Methylbut-1-ene	73	6.99
2-Methylbut-2-ene	82	14.08
Isoprene	114	10.61
Hex-1-ene	88	5.49
Cis-hex-2-ene	104	8.31
Trans-hex-2-ene	102	8.62
Alpha-pinene	68	4.51
Beta-pinene	33	3.52
Limonene	71	4.55
2-Methyl-3-butenol	-2	NA

Aromatics

VOC species	POCP[1]	MIR[2]
Benzene	10	0.72
Toluene	44	4
o-Xylene	78	7.64
m-Xylene	86	9.75
p-Xylene	72	5.84
Ethylbenzene	46	3.04
Propylbenzene	38	2.03
i-Propylbenzene	32	2.52
1,2,3-Trimethylbenzene	105	11.97
1,2,4-Trimethylbenzene	110	8.87
1,3,5-Trimethylbenzene	107	11.76
o-Ethyltoluene	73	5.59
m-Ethyltoluene	78	7.39
p-Ethyltoluene	63	4.44
3,5-Dimethylethylbenzene	104	NA
3,5-Diethyltoluene	98	8.9
1,2,3,5-Tetramethylbenzene	104	9.26
1,2,4,5-Tetramethylbenzene	100	9.26
1-Methyl-4-i-propylbenzene	75	4.44
1-Methyl-3-i-propylbenzene	88	7.10
Styrene	5	1.73

Oxygenates

VOC species	POCP[1]	MIR[2]
Formaldehyde	46	9.46
Acetaldehyde	55	6.54
Propionaldehyde	72	7.08
i-Propionaldehyde	50	NA
Butyraldehyde	70	5.97
Pentanal	71	5.08

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Oxygenates (cont.)

VOC species	POCP[1]	MIR[2]
3-Methylbutanal	41	4.97
Benzaldehyde	-19	-0.67
2-Methylbenzaldehyde	-28	NA
3-Methylbenzaldehyde	-18	NA
4-Methylbenzaldehyde	5	NA
Methanol	13	0.67
Ethanol	34	1.53
Propanol	48	2.5
i-Propanol	18	0.61
Butanol	52	2.88
i-Butanol	36	2.51
sec-butanol	40	1.36
t-Butanol	2	0.41
3-Methyl-1-butanol	44	3.16
Phenol	-5	2.76
o-Cresol	19	2.4
2,5-Xylenol	55	2.12
2,4-Xylenol	54	2.12
2,3-Xylenol	34	2.12
Cyclohexanol	45	1.95
Diacetone alcohol	29	0.6
Acetone	6	0.36
Methylethylketone	32	1.48
Methyl-i-butylketone	52	3.14
Cyclohexanone	29	1.35
Methylpropylketone	-1	2.81
Methyl formate	3	0.057
Methyl acetate	7	0.072
Ethyl acetate	19	0.63
i-Propyl acetate	21	1.07
Butyl acetate	26	0.83
n-Propyl acetate	24	0.78
Formic acid	3	0.066
Acetic acid	9	0.68
Propanoic acid	13	1.22
Dimethylether	18	0.81
Diethylether	46	3.76
Di-i-propylether	44	3.52
Ethylene glycol	33	3.13
Propylene glycol	39	2.58
2-Butoxyethanol	45	2.9
1-Methoxy-2-propanol	34	2.44
2-Methoxyethanol	29	2.93
2-Ethoxyethanol	37	3.71
Acrolein	54	7.45
Methacrolein	92	6.01
Glyoxal	22	12.5
Methylglyoxal	101	16.56

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Other VOCs

VOC species	POCP[1]	MIR[2]
Acetylene	7	0.95
Propyne	73	6.72

Halocarbons

VOC species	POCP[1]	MIR[2]
Methylene dichloride	3	0.041
Ethyl chloride	11	0.038
Tetrachloroethylene	1	0.031
Trichloroethylene	29	0.64
Ethylidene dichloride	54	0.069
Methyl chloroform	-1	0.0049
Methyl chloride	1	0.038
Cis-dichloroethylene	0	1.70
Trans-dichloroethylene	-1	1.70
Chloroform	0	0.022

MIR

The MIR scale also represents a continuum of chemical reactivity, calculated under US-specific meteorology and atmospheric conditions. It represents the increase in ozone under atmospheric model conditions that lead to the highest predicted increase in ozone per g VOC. The MIR scale is calculated using a shorter time frame (single day as compared to multi-day POCP scale). Therefore, the MIR scale may result in greater differences in absolute values between compounds which react very quickly as compared to slower reacting ones.

Utilization of the knowledge that VOCs differ in ozone formation potential varies across regulatory regions, dependent upon regulatory goals, air quality models, ability to meet air quality standards using mass-based standards, and understanding of local emissions and conditions leading to ozone formation. Limits on VOC emissions are generally mass based. In the US, reactivity-based VOC controls have been implemented in specific consumer product rules (i.e., aerosol coatings) and in the State Implementation Plan for the Houston, Texas area.

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MIR calculations for hydrocarbon solvent mixtures

The following table provides MIR calculations for hydrocarbon solvent mixtures (categorized into hydrocarbon bins based upon chemical composition and boiling point) based on a CARB contract report by Carter, 2010.

BIN	Average Boiling Point (degrees F)	Criteria	MIR Value (July 18, 2001)	MIR Value (October 2, 2010)
1	80-205	Alkanes (< 2% Aromatics)	2.08	1.42
2	80-205	N- & Iso-Alkanes (≥ 90% and < 2% Aromatics)	1.59	1.31
3	80-205	Cyclo-Alkanes (≥ 90% and < 2% Aromatics)	2.52	1.63
4	80-205	Alkanes (2 to < 8% Aromatics)	2.24	1.47
5	80-205	Alkanes (8 to 22% Aromatics)	2.56	1.56
6	>205-340	Alkanes (< 2% Aromatics)	1.41	1.17
7	>205-340	N- & Iso-Alkanes (≥ 90% and < 2% Aromatics)	1.17	1.03
8	>205-340	Cyclo-Alkanes (≥ 90% and < 2% Aromatics)	1.65	1.44
9	>205-340	Alkanes (2 to < 8% Aromatics)	1.62	1.44
10	>205-340	Alkanes (8 to 22% Aromatics)	2.03	1.98
11	>340-460	Alkanes (< 2% Aromatics)	0.91	0.70
12	>340-460	N- & Iso-Alkanes (≥ 90% and < 2% Aromatics)	0.81	0.62
13	>340-460	Cyclo-Alkanes (≥ 90% and < 2% Aromatics)	1.01	0.86
14	>340-460	Alkanes (2 to < 8% Aromatics)	1.21	0.99
15	>340-460	Alkanes (8 to 22% Aromatics)	1.82	1.57
16	>460-580	Alkanes (< 2% Aromatics)	0.57	0.52
17	>460-580	N- & Iso-Alkanes (≥ 90% and < 2% Aromatics)	0.51	0.48
18	>460-580	Cyclo-Alkanes (≥ 90% and < 2% Aromatics)	0.63	0.60
19	>460-580	Alkanes (2 to < 8% Aromatics)	0.88	0.66
20	>460-580	Alkanes (8 to 22% Aromatics)	1.49	0.95

[1] SAPRC-07: based on Carter (2010)'s work

VOC emission management

Controlling the emissions of VOCs requires a systematic approach:

- Prepare an inventory of all emission sources and quantification of the amounts emitted
- Develop an emission reduction plan based on this inventory and set priorities

Regional guidance exists for preparing emission inventories, for example:

- The European Monitoring and Evaluation Programmer (EMEP) and European Environment Agency in the EU
- EPA guidance in the US

Emission inventories and other relevant data (emission inventories of other substances, air quality modeling, etc.) are then used by local regulatory agencies to develop air quality strategies consistent with local air quality needs. Resulting air quality plans can require emission reductions for multiple substances and from varying sources, including solvent VOCs.

VOC and outdoor air quality regulations

In the quest for improved air quality, it has been shown that product-based regulations have far less impact on air quality over facility emission control regulations.

It is important to recognize that not all VOCs are equal as they can vary significantly in their potential to react with NOx and create ground-level ozone. It is more appropriate, therefore, to make choices based on VOC reactivity.

We recommend "low-ozone paints" rather than "low-VOC paints" to better protect the environment and your business.

Here is an overview of the main regulations concerning VOCs – in Europe and the US.

VOC regulations in Europe

In Europe, the three main pieces of VOC regulation are:

- National Emission Ceilings Directive
- Industrial Emissions Directive
- Paints Directive

National Emission Ceilings Directive (NEC)

In the EU, emission reduction targets are established by country in the National Emissions Ceilings (NEC) directive. This directive covers SO2, NOx, NH3, PM2.5 and NM-VOCs.

First published in 2000, the NEC Directive set emission reduction targets for 2010. For VOCs, the target was to achieve a reduction of 28% versus the level of emissions in 1990, representing a reduction of 1.1 million tons out of 3.8 million tons in 1990.

Latest NEC Directive review published end 2016

The NEC Directive was recently reviewed and the latest update published in the Official Journal on December 17, 2016:

- The VOC emission reduction target remains at 28% in 2020, meaning that no additional regulations for solvents VOCs are expected in the mid-term in the EU;
- A new VOC emission reduction target is set at 40% in 2030, i.e., 1,5 million tons, with an indicative target of 34% in 2025.

Based on updated inventories, **solvent VOCs already achieve the new 2030 target**.

Solvent VOC emissions already achieve the new target when using updated inventories. The regulatory authorities are still using original inventories developed in the 1990's to set current and future targets. In the case of solvents, the inventories are based on the use of 1 ton of solvents per year and per capita. This data is now considered to be overestimated by 30% and should be revised before the next emission target is set. The industry is working closely with the authorities to correct the base line against which future emissions targets should be set.

No impact on ExxonMobil products

The revised Directive has no impact on ExxonMobil fluids since the industry's efforts have achieved a level of solvent VOC reduction that exceeds the target set for 2020 and equals the new 2030 target when using the updated inventories.

The industry position

The European Solvent Industry Group (ESIG) welcomes the NEC revisions and supports the proposed emission reduction targets for VOCs for 2020. The European solvents industry has shown continuous commitment to improve air quality by reducing VOC emissions from solvents by more than 60% since 1990. Longer term emission reduction targets, however, should be based on comprehensive assessments of the environmental, health and economic impacts on all sectors. ESIG has been working and will keep working with EU institutions to improve air quality and to find viable solutions that benefit the environment while preserving the competitiveness of the European solvents industry:

- Ozone modeling developed by ESIG jointly with INERIS (Institut National de l'environnement et des risques) and TNO (Netherlands Organization for Applied Scientific Research) demonstrates that further solvent reduction will not result in further ozone reduction.
- ESIG's analysis of inventory of solvent emissions indicates that inventory regulators were over-estimating projected VOC emissions by 30%.
- ESIG's VOC emissions inventories paper presents its methodology for a more accurate calculation of Volatile Organic Compounds (VOCs) emissions from solvents.
- EMEP/EEA air pollutant emission inventory guidebook 2016, Technical guidance to prepare national emission inventories: provides guidance to EU Member States on how to report their emission data to the European Commission using, for the first time, the methodology recommended by the solvent industry. This will enable the European Commission to update its old data inventories.

Next step

1 July 2018: deadline for Member States to transpose the directive into national law (i.e., 18 months after the Directive's entry into force).

For further information, please contact your ExxonMobil sales representative.

Industrial Emissions Directive (IED)

The IED is the main EU instrument regulating pollutant emissions from industrial installations. The IED was adopted November 24, 2010 to replace seven previously existing directives, including former Integrated Pollution Prevention and Control Directive and VOC Solvents Emissions Directive. IED entered into force on January 6, 2011 and had to be transposed by Member States by January 2013.

Operators of industrial installations covered by the IED are required to obtain an authorization (environmental permit) from the authorities in the EU countries. The permit takes into account all environmental impacts including emissions to air, water and land, energy consumption, waste, etc. Permit conditions are based on Best Available Techniques defined for each sector. About 50,000 installations are covered by the IED.

The IED contains a separate chapter for installations and activities using organic solvents. It covers a wide range of solvent using activities, e.g., printing, surface cleaning, vehicle coating, dry cleaning and manufacture of footwear and pharmaceutical products.

- It requires installations in which such activities are applied to comply either with the emission limit values set out in the Directive or with the requirements of the so-called reduction scheme.
- Additionally, it sets out emission limit values for VOCs in waste gases and maximum levels for fugitive emissions (expressed as percentage of solvent input) or total emission limit values.

The purpose of the reduction scheme is to allow the operator the possibility to achieve by other means emission reductions, equivalent to those achieved if the emission limit values were to be applied. This could be typically achieved by substituting products with a high content of solvents for low-solvent or solvent-free products and changing to solvent-free production processes. New installations have to comply with the IED requirements at the time they start their activity.

The Paints Directive or Directive on the limitation of VOC content in certain paints and varnishes

The Paints Directive sets the VOC content limits for paints and varnishes (essentially building paints and vehicle refinishing products). It is the first European "product directive" that controls VOC content in products rather than associated emissions. Limits came into force in two phases (2007 and 2010).
Even though the former IPPC and SED regulations (now IED) contributed to the reduction of ground-level ozone, the Paints Directive was not as effective according to an ESIG study carried out in 2006. This study demonstrated that installation-related regulations are more efficient, and the best way to reduce ozone versus product-related regulation.

The study commissioned by ESIG also concluded that further VOC emissions reduction will not deliver significant ozone reduction.

The Paints Directive, which encourages conversion to heavier solvents, such as Exxsol™ D120 or water-based solvents, is ineffective in reducing ozone given the results of the 2006 ESIG study. Nevertheless, ExxonMobil offers a range of non-VOC fluids that comply with the Solvent Emission Ceilings Directive and the Paints Directive:

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Performance fluids at 20°C (EU)

Product (*)	Vapor pressure (kPa)	Initial boiling point C°	VOC status according to SED	VOC status according to the Paints Directive
Dearomatized				
Exxsol™ D220/240 Exxsol D100 ULA Exxsol D120 Exxsol D140	0.009* 0.004* 0.001* <0.001*	223 236 254 277	Non-VOC Non-VOC Non-VOC Non-VOC	VOC VOC Non-VOC Non-VOC
Isoparaffins				
Isopar™ N Isopar V	0.005* <0.001*	223 269	Non-VOC Non-VOC	VOC Non-VOC
Non-dearomatized				
Varsol™ 120	0.001*	257	Non-VOC	Non-VOC
Aromatics				
Solvesso™ 200ND Solvesso 200	0.001* 0.003*	247 237	Non-VOC Non-VOC	VOC VOC

*calculated with ExxonMobil computer model – ESIG tool

Please refer to our fact sheet providing the VOC status of all ExxonMobil fluids in Europe.

In Austria and Switzerland

Austria calls for a maximum boiling point of 200°C in its "1995 Solvents Ordinance" limiting organic solvents in a number of applications whereas Switzerland in their "VOC Ordinance" has implemented a tax scheme where VOCs refer to organic compounds with a maximum boiling point of 240°C.

For further information, consult the European Eco-Labeling scheme (2002/739/EC amending 1999/10/EC) for paints and varnishes.

See also

The ESIG vapor pressure tool: an industry standard to help assess whether hydrocarbon solvents are VOCs

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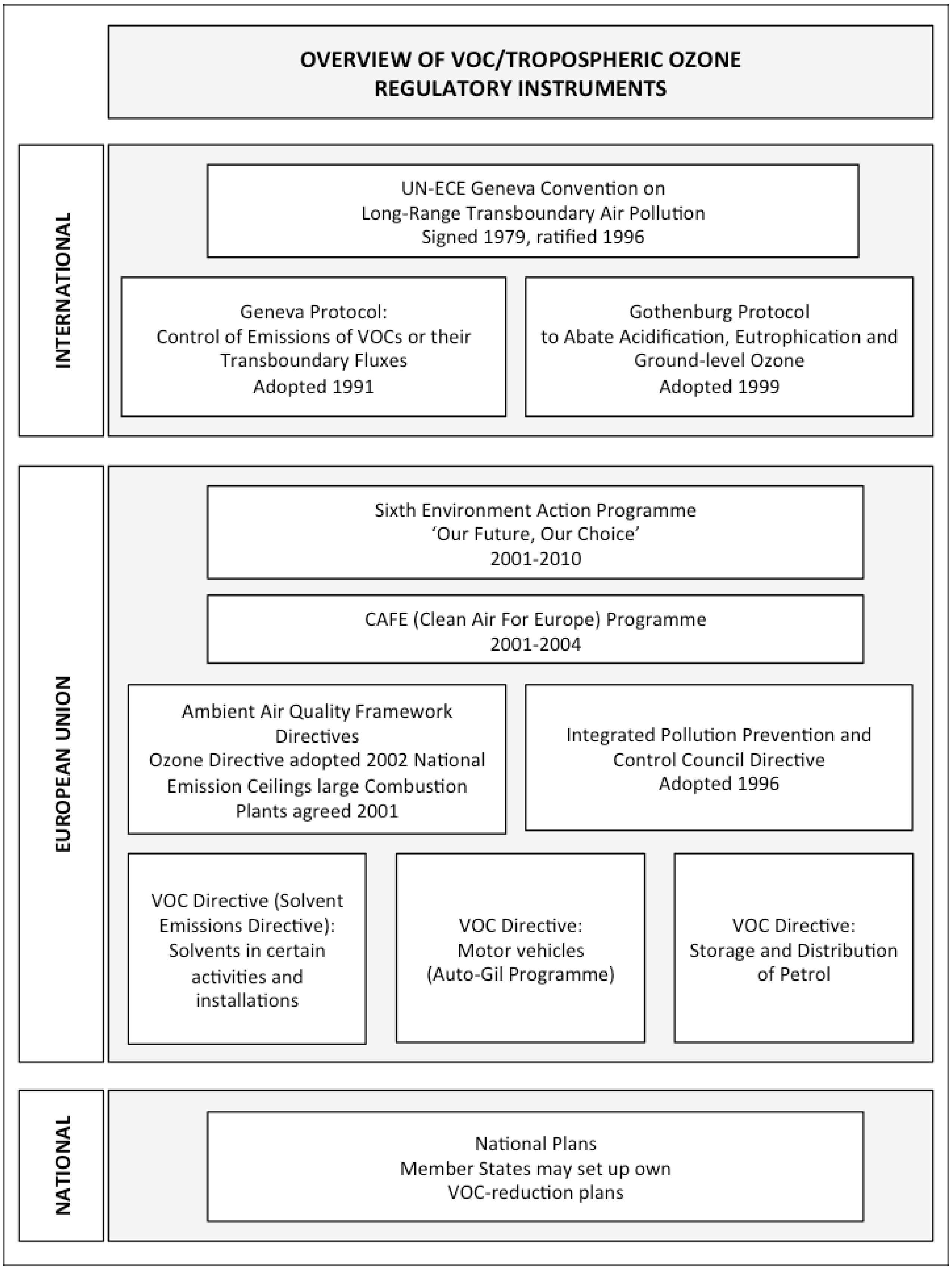
Summary of the main regulatory instrument related to VOCs/tropospheric ozone in the EU



OVERVIEW OF VOC/TROPOSPHERIC OZONE REGULATORY INSTRUMENTS

INTERNATIONAL

UN-ECE Geneva Convention on
Long-Range Transboundary Air Pollution
Signed 1979, ratified 1996

Geneva Protocol:
Control of Emissions of VOCs or their Transboundary Fluxes
Adopted 1991

Gothenburg Protocol
to Abate Acidification, Eutrophication and Ground-level Ozone
Adopted 1999

EUROPEAN UNION

Sixth Environment Action Programme
'Our Future, Our Choice'
2001-2010

CAFE (Clean Air For Europe) Programme
2001-2004

Ambient Air Quality Framework Directives
Ozone Directive adopted 2002 National Emission Ceilings large Combustion Plants agreed 2001

Integrated Pollution Prevention and Control Council Directive
Adopted 1996

VOC Directive (Solvent Emissions Directive): Solvents in certain activities and installations

VOC Directive:
Motor vehicles
(Auto-Gil Programme)

VOC Directive:
Storage and Distribution of Petrol

NATIONAL

National Plans
Member States may set up own
VOC-reduction plans

Instrument	**Geographical scope**	**Dates**
UN-ECE Geneva Convention on long-range transboundary air pollution	International	Signed November 1979 Ratified by 40 countries June 1996
UN-ECE Geneva protocol concerning the control of emissions of VOCs or their transboundary fluxes	International	Adopted 1991. Signed by 22 countries and the EU
UN-ECE Gothenburg Protocol to abate acidification, eutrophication and ground level ozone	International	Adopted 1999
Fifth Environmental Action Programme "Towards Sustainability"	European Union	Programme ran from 1992-2000
Council Directive on Integrated Pollution Prevention and Control	European Union	Adopted in 1996
Environment Council Framework Directive on ambient air quality assessment and management	European Union	Adopted in 1996
Directive of the European Parliament and of the council relating to ozone in ambient air	European Union	Adopted in 2002
Directive of the European Parliament and of the council on national emission ceilings for certain atmospheric pollutants	European Union	Adopted in 2001
Directive of the European Parliament and Council relating to measures to be taken against air pollution by emissions from motor vehicles and Amending Directives 70/220/EEC and 70/156/EEC	European Union	Adopted in 1996
Council Directive on the control of VOC emissions resulting from the storage of petrol and its distribution from terminals to service stations	European Union	Adopted in 1994
Council Directive on the limitation of emissions of organic compounds due to the use of organic solvents in certain processes and industrial installations	European Union	Adopted in 1999
Sixth Environmental Action Programme "Our Future, our Choice"	European Union	Programme ran until 2010
The Clean Air for Europe Programme	European Union	2001-2005
Directive of the European Parliament and of the Council on the limitation of emissions of volatile organic compounds due to the use of organic solvents in certain paints and varnishes and vehicle refinishing products	European Union	Adopted in April 2004

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VOC regulations in USA

In the USA, the key pieces of regulation are at national level. However, some states do incorporate their own legislation.

Clean Air Act (CAA) of 1970, amended in 1977 and 1990

In the United States, VOC controls in air are set out in the Clean Air Act (CAA) of 1970, amended in 1977 and 1990. The goal of the CAA is to reduce VOC emissions and implement abatement strategies for regions where ozone levels are high. Such strategies include reduction of automobile use, VOC emission reduction, and seasonal shifts to reformulated gasoline with high oxygenate concentrations. Currently the Clean Air Act mandates that MACT (Maximum Achievable Control Technology) should be used to help ensure attainment of the required ozone air quality standards. Human health risk assessments are to be performed on the remaining VOC emissions by the US Environmental Protection Agency (EPA). Results of these risk assessments could stimulate further regulatory action.

It should be noted that the US has taken primarily an EQO/EQS approach and is applying MACT where this is required. This approach helps to ensure the most effective use of resources.

National Ambient Air Quality Standards for ozone

The US has also set National Ambient Air Quality Standards for ozone. The current standard for both human health (primary standard) and ecological endpoints (secondary standard) is set at the level of 0.070 ppm for an 8-hour averaging time, with a form as an annual fourth highest daily maximum 8-hour concentration averaged over three years.

At the Federal level, the US EPA currently uses ethane as a benchmark for VOC exemptions based on reactivity considerations. The state of California has incorporated MIR into aerosol coatings regulations.

Low vapor pressure (lvp) fluid options for consumer products

Concerns around air quality and ozone continue to drive consumer product formulation decisions. In order to help our customers meet the ever-changing regulations, ExxonMobil markets several LVP-VOC fluids for consumer product applications that meet the low vapor pressure requirement defined by the California Air Resources Board (CARB) and the U.S. EPA as:

- Having a vapor pressure of less than 0.1 mm Hg at 20° C, or
- Consists of more than 12 carbon atoms, if the vapor pressure is unknown,
- Boils or distills >216° C (this additional criterion is included in CARB's regulation)

Product	CAS number	Compliance with LVP Criteria
Exxsol™ D 95 fluid	64742-47-8	100%
Exxsol D 110 fluid	64742-47-8	100%
Exxsol D 130 fluid	64742-46-7	100%
Isopar™ M fluid	64742-47-8	100%
Isopar V fluid	64742-46-7	100%
Aromatic 200 / ND / ULN	64742-94-5	100%

For additional information see: National Volatile Organic Compound Emission Standards for Consumer Products, or **contact your sales representative or your distributor**.

Safety data sheets

Safety data sheets

The online data base of ExxonMobil Chemical safety data sheets is accessible below.

Access data sheets here

ExxonMobil Chemical has a strong commitment to product safety. We are dedicated to minimizing adverse risks and impacts associated with the manufacture, use, and disposal of our products.

During the development of and prior to marketing our products, we assess safety, health, and environmental (SHE) aspects as well as compliance with product safety legislation, both where the products are made and in their intended markets. Rigorous assessments required by government authorities are conducted and updated as new information becomes available to assure the safety of our products.

Through safety data sheets (SDS), we provide this information to those who transport, use, and dispose of our products, including appropriate uses, potential health and environmental effects, personal protection and exposure controls, first aid measures, and disposal considerations.

SDSs are provided to our customers via an automatic system, the internet, or work procedures. The latest revision of the SDS should always be consulted. According to our policy, we will provide them with an SDS of any of our chemicals products even where this may not be required by law.

The GHS standard, organized in 16 sections, is the standard in most areas:

- In the EU, it was adopted by REACH.
- In Asia Pacific, it is widely used.
- In the US, the SDS format is being aligned with GHS recommendations as GHS is implemented.

Slight variations between countries in the format or content of an SDS may occur to accommodate specific local legal requirements, e.g., if a product is classified in one country but not in another. A significant difference in the EU SDS lies in the fact that the EU SDS includes exposure scenarios.

The EU SDS with an attached exposure scenario is typically referred to as an extended safety datasheet or ext-SDS:

- Overview of the difference between an SDS prior to REACH and an ext-SDS
- Example of an ext-SDS

The sections in right hand navigation lead you to a summmary of the information presented in each section of an SDS. More details are available in our User's Guide to Safety Data Sheets.

Section 1: Product and company identification

Information overview:

- Identification of the product;
- Chemical family;
- Product description;
- Intended uses;
- Supplier information;
- Emergency telephone number(s).

The safety data sheet (SDS) shows the chemical family (e.g., solvent, plasticizer, etc.) to which the product belongs, together with a product description, its appearance and physical state. It indicates also the most important or common known uses of the substance or preparation.

The name, address and telephone numbers of appropriate ExxonMobil Chemical affiliates are given for further information or in the case of an emergency.

Click here to see section 1 of a real SDS.

Safety data sheets »
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Section 2: Hazard identification

Information overview:

- Health hazards;
- Environmental hazards;
- Physical and chemical hazards/fire and explosion hazards;
- Classification of the substance or mixture;
- Labeling information.

This section describes the hazard(s) of the product (substance or mixture) and the appropriate warning information (signal word, hazard statements and precautionary statements). More detailed information on these hazards is provided elsewhere in the safety data sheet (SDS). All necessary information on classification and labeling is also displayed within this section.

Click here to see section 2 of a real SDS.

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Section 3: Composition and information on ingredients

Information overview:

- CAS number (for substances only);
- Reportable hazardous components;
- GHS classifications.

The information in this section will identify the product, including reportable impurities and stabilizing additives which are themselves classified and contribute to the classification of the product.

For products that are **mixtures**, information on the chemical identity and concentration or concentration ranges of all hazardous substances present above their cut-off levels will be provided.

Click here to see section 3 of a real SDS.

Section 4: First aid measures

This section describes the initial care that can be given by an untrained responder without the use of sophisticated equipment. Instructions will state if medical attention is required and its urgency. The measures provided in this section are recommendations for immediate first aid treatment for the identified routes of exposure:

- **Inhalation**: the breathing in of fumes, mists, vapours or dusts.
- **Dermal (skin contact)**, with two possible effects that may occur:
  - Local effects such as skin irritation arising from the direct action of the product at the point of first contact on the skin.
  - Systemic effects, i.e., damage caused to tissues due to the product penetrating the skin barrier and passing into the body.
- **Eye**: this is normally confined to local eye effects such as irritation or burns, but there are a few substances which can be absorbed into the body through the eye and these may cause systemic toxic effects.
- **Ingestion**: swallowing the product.

Click here to see section 4 of a real SDS.

Section 5: Fire fighting measures

Information overview:

- Extinguishing media;
- Fire fighting;
- Flammability properties;
- Specific considerations.

This section provides general guidance on firefighting and on appropriate extinguishing agents to assist competent personnel at the incident. In case hazardous by-products are likely to be released by the fire or firefighting methods, the precautions to be observed by firefighters are detailed.

Click here to see section 5 of a real SDS.

Section 6: Accidental release measures

Information overview:

- Notification procedures;
- Protective measures;
- Spill management;
- Environmental precautions.

This section provides general recommendations on the appropriate response to spills, leaks, or releases, to prevent or minimize any adverse effects on persons, property and the environment.

Click here to see section 6 of a real SDS.

Section 7: Handling and storage

Information overview:

- Storage temperature;
- Transport temperature;
- Loading/unloading temperature;
- Storage/transport pressure;
- Electrostatic accumulation hazard;
- Usual shipping containers;
- Materials and coatings suitable/unsuitable;
- Storage/handling general notes;
- Additional warnings.

This section provides information on the temperature at which the product should be stored, transported or transferred, as well as other relevant data to enable safe handling, transportation and storage. The aim is to assist the employer in devising suitable working procedures and organizational measures. This section also provides general guidance concerning materials and coatings that are suitable or unsuitable for storage and transfer operations.

Click here to see section 7 of a real SDS.

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Section 8: Exposure controls, personal protection

Information overview:

- Engineering control measures;
- Occupational exposure limits;
- Derived no effect/minimal effect level (EU);
- Predicted no effect level (EU);
- Personal protective equipment.

The recommendations and data in this section are aimed at achieving good industrial hygiene and environmental control practices at work. This section provides the exposure limit values that are applicable and the related exposure control measures that are recommended. In the case of EU SDSs, the derived no effect/minimal effect level and predicted no effect level will also be given.

The precautions given in this section apply only to the product as originally supplied. Mixing the product with other materials may alter the precautions.

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Section 9: Physical and chemical properties

This section describes empirical physical and chemical property data relating to the product and includes information such as:

- Appearance;
- Physical state;
- Melting point, etc.

These values are "typical" only and should not be construed as the specifications of the product being sold.

Click here to see section 9 of a real SDS.

Section 10: Stability and reactivity

Information overview:

- Stability and conditions to avoid;
- Hazardous polymerisation and conditions to avoid;
- Incompatible materials;
- Hazardous decomposition products;
- Hazardous combustion products.

This section describes the stability of the product and the potential for hazardous reactions occurring under certain conditions of use and also if released into the environment.

Click here to see section 10 of a real SDS.

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Section 11: Toxicological information

Information overview:

- Acute toxicity hazards through inhalation, skin contact , eye contact, ingestion;
- Sensitization;
- Aspiration;
- Germ cell mutagenicity;
- Chronic toxicity/carcinogenicity;
- Reproductive/developmental toxicity;
- Specific target organ effects;
- Other information.

This section is used primarily by medical professionals, occupation health and safety professionals, and toxicologists. It provides information on the health hazards of the material. If necessary, it also makes reference to specific health effects of certain components.

The information provided in this section provides a description of the possible health hazards of the product. The toxicological information also provides the basis for the advice found in "First- aid measures" (section 4), and "Exposure controls and personal protection" (section 8).

Reference may also be given to substances identified as carcinogens and identified on authoritative regulatory lists.

Click here to see section 11 of a real SDS.

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Section 12: Ecological information

Information overview:

- Toxicity;
- Persistence and degradability;
- Bioaccumulative potential;
- Mobility in soil;
- Persistence, bioaccumulation and toxicity for substances;
- Other adverse effects.

The information provided in this section describes the possible effects, behaviour and environmental fate of the product in air, water and/or soil.

Click here to see section 12 of a real SDS.

Section 13: Disposal considerations

Information overview:

- Disposal recommendations;
- Regulatory disposal information.

Waste treatment methods are governed in many cases by local and national legislation. Before disposal, a specialist should be consulted.

Click here to see section 13 of a real SDS.

Section 14: Transport information

Information overview:

- Land (railroad/road, such as RID/ADR):
  - RID/ADR class, item;
  - Danger number;
  - Danger label;
  - Transport document name;
  - Tremcard product name;
  - Empty containers;
  - Substance ID number.

- Inland waterways (such as ADN/R):
  - ADN/R class;
  - UN number;
  - Transport document name.

- Sea (IMDG):
  - UN number;
  - IMDG class or division;
  - Packaging group;
  - EMS number;
  - Marine pollutant status;
  - Risk label;
  - Subsidiary risk.

- Air (ICAO/IATA) ICAO/IATA class:
  - Packing group;
  - UN number.

This section covers the classification and labeling for transport by road/rail, barge, sea, and air. It provides also, if and when needed, the references to the sections of the relevant transport regulation.

Click here to see section 14 of a real SDS.

Section 15: Regulatory information

Information overview:

- Regulatory status and applicable laws and regulations;
- Safety, health, and environmental regulations/legislation specific for the substance or mixture.

This section provides safety, health, and environmental regulations or legislation specific for the substance or any component presenting a health or environmental hazard.

Click here to see section 15 of a real SDS.

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Section 16: Other information

Information overview:

- Revision summary;
- Additional comments.

Information that is not covered in the previous sections that may have an effect on or an important relationship to safety, health or the environment is added here.

Click here to see section 16 of a real SDS.