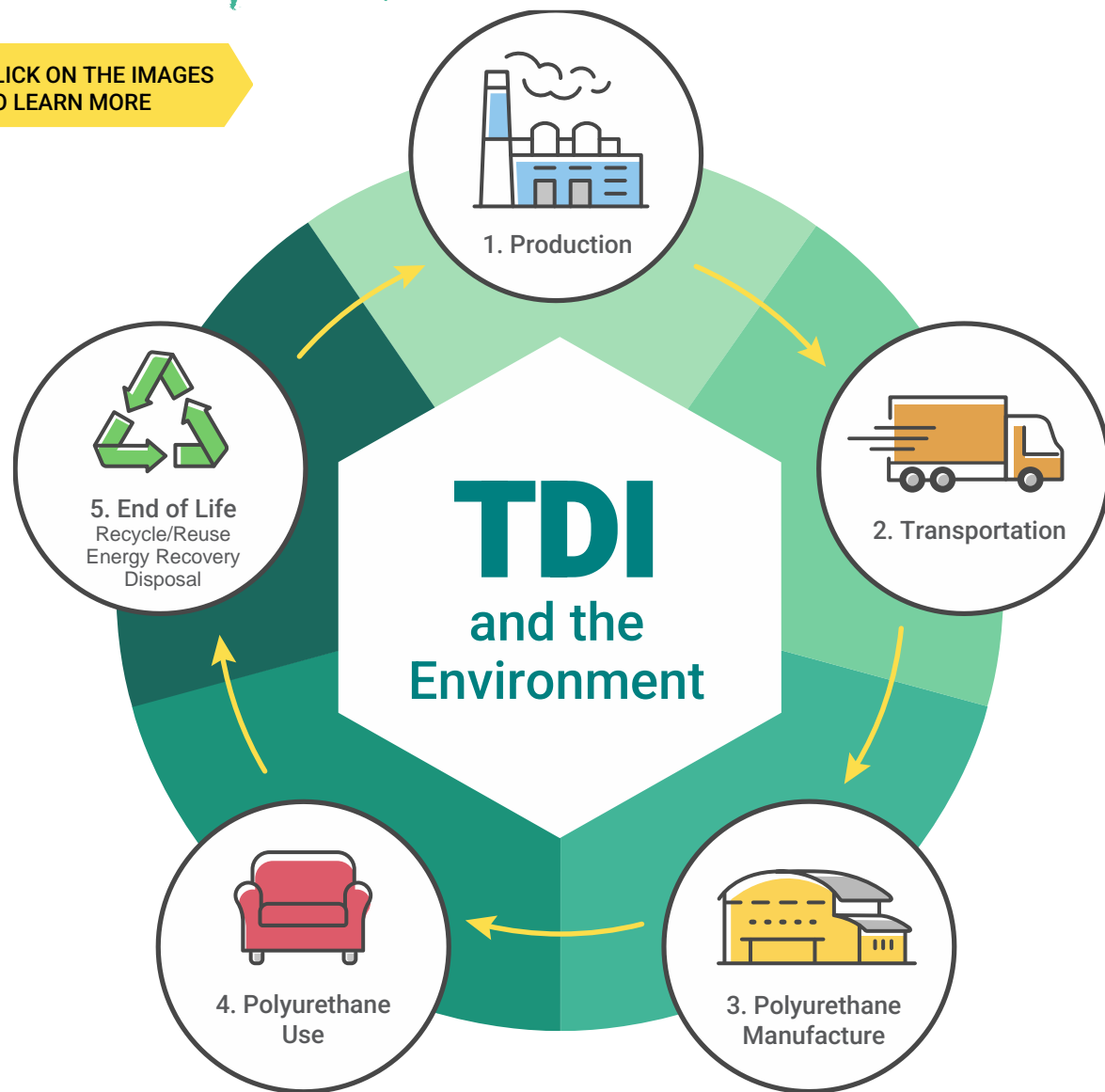




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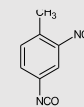


Abstract

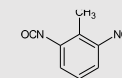
Toluene diisocyanate (TDI) is a versatile chemical intermediate used in the manufacture of a variety of polyurethane materials and has an estimated global production exceeding one million metric tons/yr. This substance is highly reactive with water - even with the water vapor in air - which along with its potential health hazards compels very strict handling and containment during its manufacture, transportation, formulation, and application.

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What is TDI?



2,4-Toluene Diisocyanate (2,4-TDI)



2,6-Toluene Diisocyanate (2,6-TDI)

Toluene diisocyanate (TDI) is a reactive chemical intermediate used primarily in the manufacture of polyurethanes.

[Click to read more.](#)

TDI in the Atmosphere

Photolysis

Oxidation to CO₂, H₂O, NO_x

TDI in the Aquatic Environment

Hydrolysis

TDA in Water/Sediment
Polyurea in Sediment

TDI in Soil

Hydrolysis

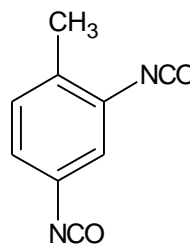
Polyurea in Soil
TDA in Soil

ABSTRACT

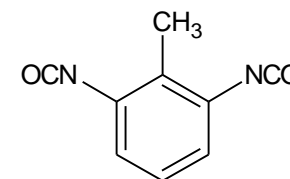
Toluene diisocyanate (TDI) is a versatile chemical intermediate used in the manufacture of a variety of polyurethane materials and its estimated global production exceeds 1MM tons/yr (Carvajal-Diaz, 2015). This substance is highly reactive with water- even with the water vapor in air- which along with its potential health hazards compels very strict handling and containment during its manufacture, transportation, formulation, and application. These control measures ensure that only a small fraction of the large production volume could be emitted to the environment. This presentation summarizes existing information on the fate and potential effects of TDI which could be expected when its emission to air, water, or soil may occur. The reaction of TDI with water (hydrolysis) present in the air, water, and soil converts the substance to solid inert polyureas. Much like the polyurethanes which are manufactured from TDI, these polyureas are stable in the environment and on disposal have no adverse impact on domestic waste handling processes, landfills, or incineration.

WHAT IS TDI?

Toluene diisocyanate (TDI) is a reactive chemical intermediate used primarily in the manufacture of polyurethanes. The reactivity of this substance is derived from the two isocyanate (NCO) functional groups associated with the TDI molecule. The majority of TDI is produced and used in a liquid state as a mixture of the 2,4- and 2,6-TDI isomers in fixed ratios of 80:20 or 65:35 (wt:wt). Most of the TDI in commerce occurs as the 80:20 (2,4-:2,6-; wt:wt) mixture. Representative chemical structures of the 2,4- and 2,6-TDI isomers are shown below:



2,4-Toluene Diisocyanate (2,4-TDI)



2,6-Toluene Diisocyanate (2,6-TDI)

[Next](#)

TDI PHYSICAL-CHEMICAL PROPERTIES

Table 1. Summary of Key Physical-Chemical Properties of TDI Substances

PROPERTIES OF 80:20 TDI	VALUE
Vapor Pressure (@ 20°C or 68 °F)*	1.5 mPa (0.01 mmHg)
Saturated Vapor Concentration (@ 20°C or 68 °F)	107 mg/m ³ 14 parts per million (ppm)
Boiling Point (@ 101.3kPa, 760 mmHg)	252 – 254 °C (485.6 – 489.2°F)
Freeze Point	9.5 °C (49.1 °F)
Relative Density (@ 20°C or 68 °F)	1.22
Water Solubility (@ 20°C or 68 °F)	Insoluble; hydrolyzes in water

* Vapor pressures and saturated vapor concentrations at other temperatures are reported in Pemberton (2001)

PROPERTIES OF 65:35 TDI	VALUE
Vapor Pressure (@ 20°C or 68 °F)*	1.4 mPa (0.01 mmHg)
Saturated Vapor Concentration (@ 20°C or 68 °F)	107 mg/m ³ 14 parts per million (ppm)
Boiling Point (@ 101.3kPa, 760 mmHg)	253 – 255°C (487.4 – 491 °F)
Freeze Point	4 °C (39.2 °F)
Relative Density (@ 20°C or 68 °F)	1.22
Water Solubility (@ 20°C or 68 °F)	Insoluble; hydrolyzes in water

MANUFACTURING AND USES



TDI PRODUCTION EMISSIONS

The production of TDI is carried out in closed equipment with emission controls on all vents. Emissions of TDI to the atmosphere are therefore very low. For example, for the year 1997 emissions to air and water associated with TDI production sites in Europe were $< 0.000005\%$ of annual production. Reported estimates of emissions to air and water associated with TDI production in the U.S. are also a negligible fraction of total production (US EPA, 2021).



POLYURETHANE MANUFACTURING EMISSIONS

Polyurethanes are produced by reacting diisocyanates such as TDI with polyols; other chemicals such as catalysts, surfactants, antioxidants, and flame retardants may be included in the formulation to obtain targeted properties of the polyurethane materials. A significant use of TDI is in the production of flexible slabstock foam, from which emission losses to the atmosphere have been estimated at < 25 grams per ton of TDI used (Chapman, 1994), equivalent to an approximate 0.0028% emission rate. Measured stack vent concentrations of TDI for European flexible foam plants were found to be in the range of 0.15 to 6 mg/m^3 ($0.02 - 0.8 \text{ ppm}$), which is well below the saturated vapor concentration and indicating that TDI emissions occur in the vapor (not aerosol) phase



POLYURETHANE USE

TDI is used in the production of polyurethanes, primarily for flexible foam. 'Slabstock' foam applications include bed mattresses and furniture cushions, carpet underlay, as well as cushioning in packaging applications. Molded flexible foam applications include automotive and aircraft seating as well as bed pillows. Minor amounts of TDI are used in the manufacturing of coatings, sealants, adhesives, and elastomers.

TDI in the Atmospheric Environment

ATMOSPHERIC FATE OF TDI

As is the case for most aromatic organic substances, the reaction with photochemically-generated hydroxyl radical is the most important atmospheric degradation process affecting the fate and lifetime of TDI in the atmosphere. The estimated atmospheric half-life of TDI is about one day when typical daylight hours (12 hr) and hydroxyl radical concentrations are assumed (Tury et al., 2003). Because the atmospheric concentrations of both water vapor and TDI are very low, hydrolysis of TDI is not consequential to its fate and lifetime in the atmosphere, as has been experimentally demonstrated (Holdren et al., 1984). Reaction pathways that could lead to the formation of aromatic diamines from the atmospheric reaction of aromatic diisocyanates with OH radicals are extremely unlikely (Pfeifle et al., 2021)

Environmental chamber experiments and computer model calculations were carried out to assess the atmospheric ozone formation potential of 2,4- and 2,6-TDI (Carter et al., 1997). The major conclusion is that emissions of TDI are unlikely to have a positive effect on ozone formation under any atmospheric conditions, and thus it should not be an ozone precursor or contributor to urban smog formation.

TRANSPORTATION



TRANSPORTATION

Large quantities of TDI are routinely transported over road, rail, and sea in a variety of container types and sizes. Even the smallest spillages of TDI during its transport are rare; however, this is perhaps the most plausible mode of TDI emission to the soil or water compartments since other modes are prevented through the strict emission controls implemented during manufacture, formulation, and end-use life cycle stages. In the unlikely event of a spillage to the aquatic or soil environments, TDI reacts (hydrolyzes) rapidly to form inert polyureas which can usually be collected and disposed as solid waste. The learnings derived from a limited number of past TDI spillage incidents have indicated no evidence for long-term impacts to the environment and biota; immediate physical impacts of the spill are most severe (e.g., due to potential physical contact of people, environment, and wildlife with unreacted TDI liquid and vapor) (Allport et al., 2003).



TDI NEUTRALIZATION

TDI residues remaining in emptied containers can be neutralized by application of water-based solutions which promote the polyurea formation reaction. A simple formulation of water, nonionic surfactant (2% wt.) and monoethanolamine (MEA; 1% wt.) was optimized for neutralization of TDI in emptied 200 L steel drum containers (Hugel and West, 2014). It was shown that relatively small volumes (~ 2 L) of neutralization solution are necessary, and that spent neutralization solution could be disposed via a domestic sewage treatment plant (STP) with no expected detrimental effects to the wastewater treatment microorganisms or to aquatic life in the STP effluent (Allmendinger et al., 2014). It was also shown that a household laundry detergent which contains nonionic surfactant and MEA could be diluted in water to approximate these optimum concentrations and is similarly safe and effective in TDI neutralization. Neutralization should never be applied in a sealed container, and all appropriate regulations should be followed when disposing of neutralized containers and spent neutralization solution.

TDI POLYUREAS



FORMATION

Various substituted polyureas are formed during reaction of TDI under heterogeneous mixing with water. The mono-ureas represent the first intermediate products in the stepwise formation of polyurea which is the ultimate end-product of such hydrolysis reactions. The isocyanato-terminated ureas are transient species. To the extent soluble, the terminal isocyanate (NCO) groups hydrolyze in water. Like isocyanates and their corresponding amines, the terminal NCO and amino (NH₂) groups of the ureas will react to form oligo- and poly-ureas as the final hydrolysis product (see '[HYDROLYSIS](#)' slide for structures). TDI polyureas are inert and insoluble in water and most organic solvents. The photo at the left shows TDI polyureas formed by stirring 50 g/L of TDI (80:20 2,4-TDI: 2,6-TDI) in distilled water for 14 days.

FATE AND TOXICITY

The half-time for hydrolysis of TDI-polyurea at 25 degrees C in deionized water has been estimated to range from about 18,000 to 300,000 years, depending on the kinetic assumptions made (Sendijarevic *et al.*, 2004). The half-times for hydrolysis at buffered pH levels of 4, 7, and 9 were within a factor of 2 of those in deionized water. The additional data in Table 3 further supports the characterization of TDI polyureas as essentially non-toxic and inert.

Table 3. Summary of key environmental fate and acute hazard properties of amine- and isocyanate-terminated mono-ureas of TDI

Property	Method	Endpoint ¹	NCO-terminated mono-urea of TDI	NH ₂ -terminated mono-urea of TDI
CASRN			Not available	Not available
<i>Acute toxicity information (from Loddenkemper et al., 2019 and Steinhoff, 1973)</i>				
Ready Biodegradability	OECD 301F		Not readily biodegradable	
72 h Algae Growth Inhibition [mg/L]	OECD 201	E _r L ₅₀ / E _r C ₅₀ NOEL _r / NOEC _r	>100 / - >100 / -	>100 / - >100 / -
48 h Daphnia magna Immobilization [mg/L]	OECD 202	EL ₅₀ EC ₅₀	>100 -	- >100
96 h Danio rerio Lethality [mg/L]	OECD 203	LL ₅₀ EC ₅₀	>100 -	- >100
Acute oral toxicity in rat [mg/kg body weight]		LD ₅₀	Not determined	>15,000

¹Endpoint Key:

E_rC(L)₅₀ – Median Effective Concentration (Loading Rate) [causing 50% reduction in growth rate of exposed population]

NOEC(LR) – No Observed Effect Concentration (Loading Rate) [highest loading rate showing no effects of exposed population]

EC(L)₅₀ - Median Effective Concentration (Loading level) [showing the measured effect in 50% of tested individuals]

LL(D)₅₀ - Median Lethal Loading Rate Dose) [causing mortality in 50% of exposed population]

TDI Hydrolysis

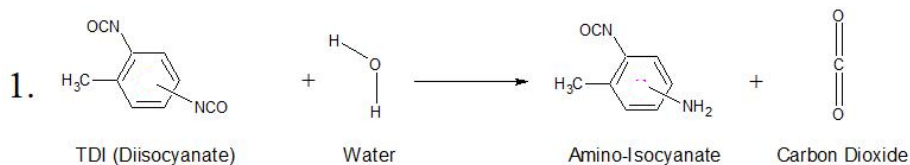
Hydrolysis (reaction with water) is the most important process affecting the fate and potential hazards of TDI in the environment. A basic understanding of this reaction is necessary to understand and interpret the following sections on **TDI IN THE AQUATIC ENVIRONMENT, TDI IN SOIL, SPILLAGE SIMULATION STUDY, and TDI ECOTOXICITY**. This reaction occurs between water and the two isocyanate (NCO) functional groups of TDI as shown in the following (simplified) sequence of reaction steps:

Note: The rate of reaction between isocyanate and amine (Steps 2 and 4) has been determined to be ~ 10,000 times faster than that between isocyanate and water (Steps 1 and 3). Step 2 has a much higher probability to occur than Step 3. The practical implications of this complex hydrolysis reaction are further illustrated in **TDI IN THE AQUATIC ENVIRONMENT**.

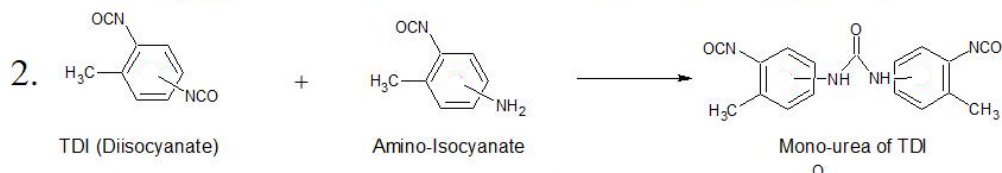
A short, animated presentation of hydrolysis is available at the following [LINK](#).

[Return to Start](#)

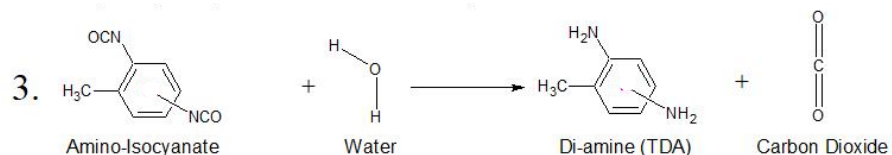
Step 1 (the amine-forming step) converts one of the isocyanate (NCO) functional groups to an amine group (via a carbamic acid intermediate, not shown) and releases carbon dioxide.



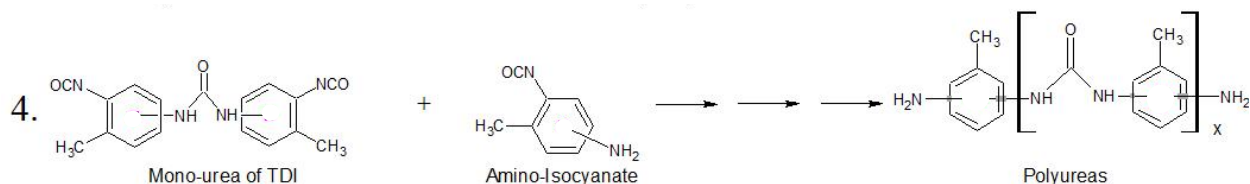
Step 2 (the urea-forming step) combines the amine group formed in Step 1 with an isocyanate group of another molecule of TDI or of the amino-isocyanate intermediate to form a mono-urea.



Step 3 (the diamine-forming step), the isocyanate group of the amino-isocyanate formed in Step 1 reacts with water to form a di-amine (i.e., TDA). Since formation of diamine requires simultaneous conversion of both isocyanate groups, this step has a low probability to occur under most realistic environmental conditions.



Step 4 (the polyurea-forming step), the isocyanate groups associated with urea formed in Step 2 continue to preferentially react with amine groups formed in Step 1, and polyureas are formed with continually increasing molecular weight while amine groups are consumed as quickly as they are formed.

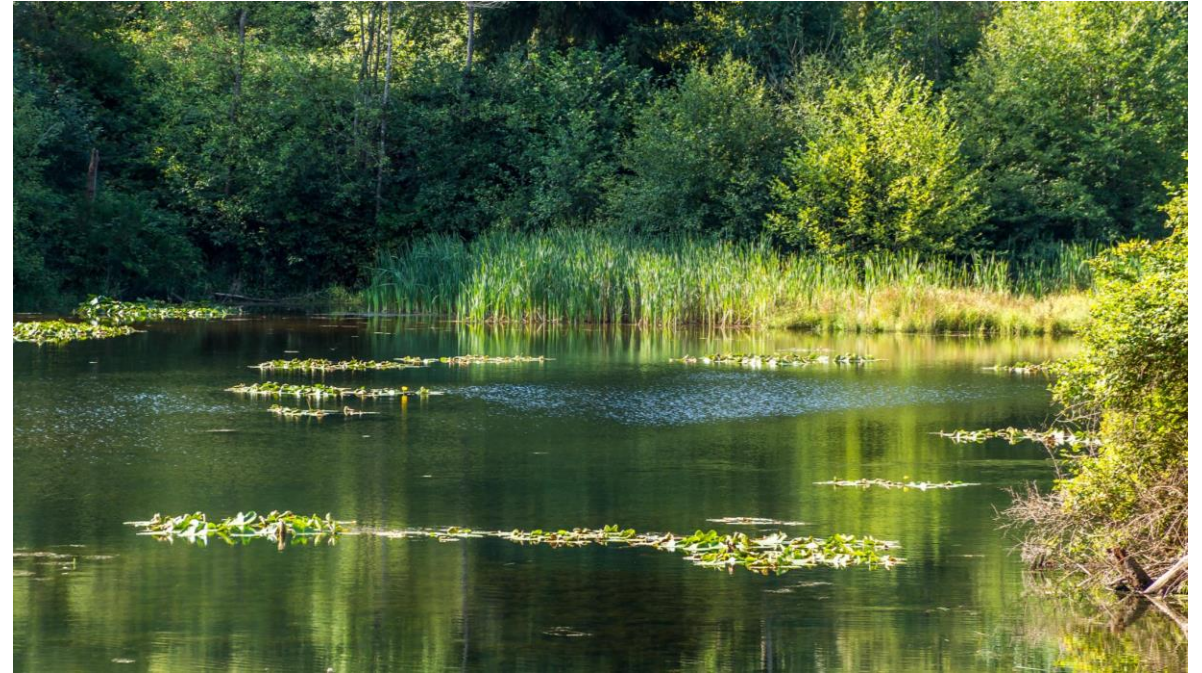


SPILLAGE SIMULATION STUDY

A constructed pond (mesocosm) study was designed and conducted to simulate the potential short- and long-term effects of a liquid polymeric methylene diphenyl diisocyanate (pMDI) spillage into an aquatic ecosystem (Heimbach et al., 1996). Since TDI is a structurally similar liquid aromatic polyisocyanate substance, the findings of this study can illustrate the expected behaviour of a TDI spillage to water as well.

Three interconnected and identical artificial ponds (4.2 m³ volume, 1.3 m deep) were constructed which contained lake sediments and circulated well water. After populations of various algae, plankton, fish, and plant species were established and equally distributed among them, the ponds were isolated and liquid pMDI was added to two of the ponds in amounts equaling 1 or 10 g/L while the third pond served as a control. Aquatic chemistry and species population densities were monitored for 112 days following these simulated pMDI spills. There were no direct effects observed on the pelagic species (fish, plankton) and only temporary effects were noted with the sediment-dwelling organisms due to physical obstruction of the sediment surface by polyureas formed. Evolution of CO₂ from pMDI hydrolysis caused a temporary drop in water pH and an associated stimulation of aquatic plant and algae growth. After 112 days, water quality and biotic population parameters were essentially equal across all three ponds, and all the applied pMDI mass could be recovered as the converted polyurea solids.

Analytical monitoring indicated that MDI and MDA were not detectable in the water (< 0.01 mg/L) and fish tissues (< 0.5 mg/kg MDI, < 1.4 mg/kg MDA) over the course of this study. These results are consistent with the observations of MDI and TDI behaviour and minimal associated impacts observed with a limited number of actual spillages and demonstrate that such events will have no long-term effects on the environment.



TDI in the Aquatic Environment

TDI is a hydrophobic substance which will remain as a viscous oily droplets when introduced to water. Since the TDI substances have higher density than water (Table 1), they tend to sink through the water column and can coalesce into larger droplets or clusters as was observed with pMDI in a spillage simulation study. As the TDI immediately begins to hydrolyze, carbon dioxide is released and a coating of polyurea will form over the surface of these particles or droplets. As the hydrolysis reaction continues, this coating continues to grow thicker until the original particle or droplet of TDI is fully converted to a polyurea particle.

This hydrolytic conversion of TDI to polyureas can take from a few hours to several days, depending on the size of the TDI droplets, water temperature, and degree of mixing (see Figures 1a-b). As shown in Figure 1c, under controlled laboratory conditions where small amounts of TDI can be combined with large volumes of water, small amounts of toluene diamine (TDA) can be formed as a by-product of hydrolysis. The yield of TDA generally increases with increased loading rate and degree of mixing, yields of TDA ranging from < 0.08% (unstirred) to ~ 0.39 % (vigorous stirring) conversion of the initial TDI mass (Yakabe et al., 1999). If a small amount of TDI is first dissolved in an organic solvent and then vigorously mixed into water, the conversion of TDI to TDA can theoretically approach 100%. However, there are no such reaction conditions associated with known or plausible modes of TDI emission to the environment

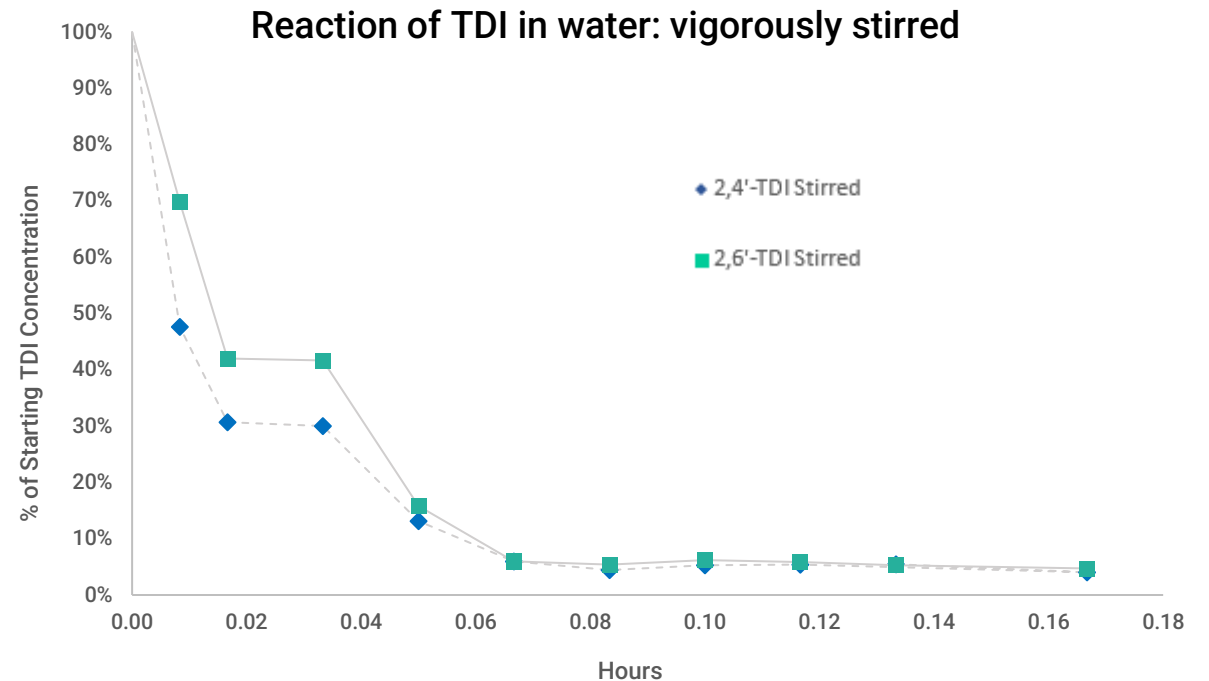
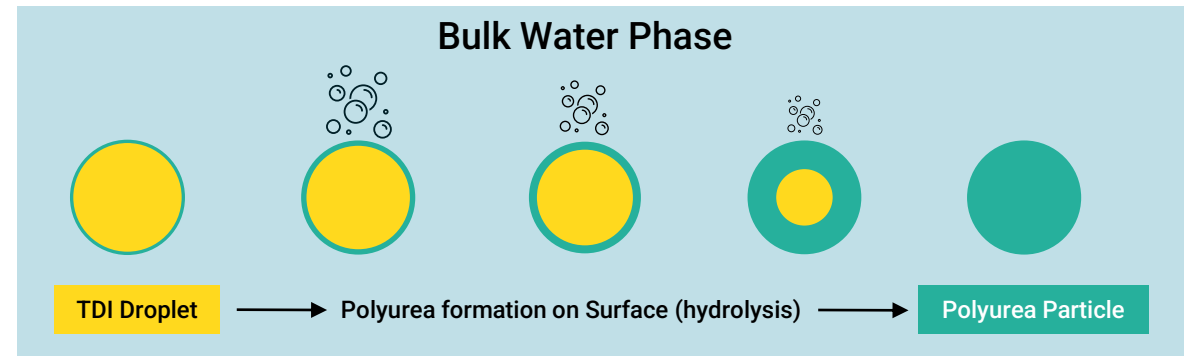


Figure 1a. Hydrolysis of the 2,4- (80%) and 2,6-TDI (20%) components of 80:20 TDI in water (28 mg/L) under vigorously stirred conditions.

TDI in the Aquatic Environment

Reaction of TDI in water: unstirred

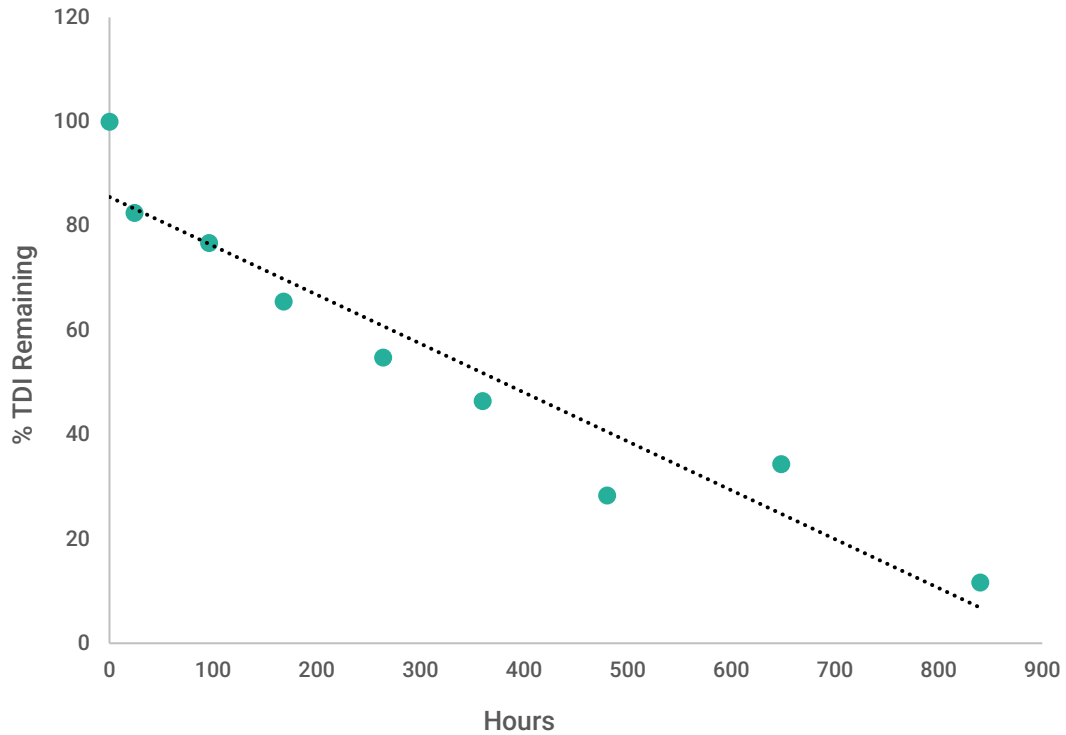


Figure 1b. Hydrolysis of 80:20 TDI in water under unstirred conditions.

Conversion of TDI to TDA in Water

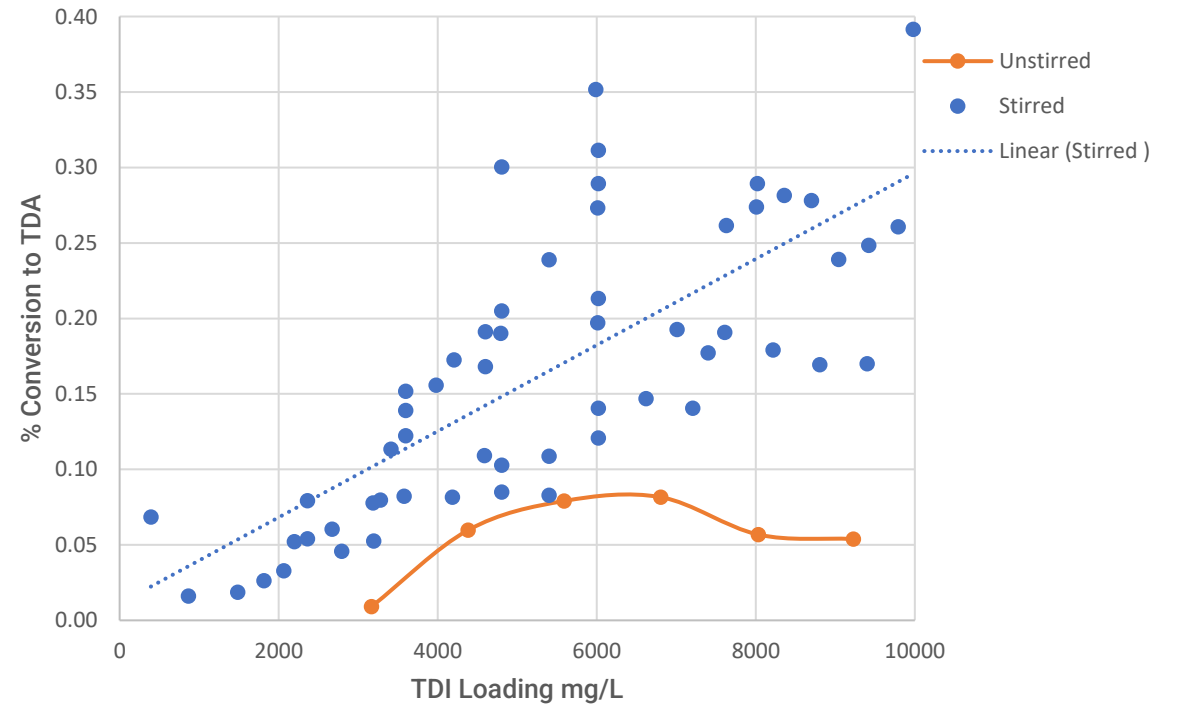


Figure 1c. Formation of toluene diamine (TDA) as a function of 80:20 TDI loading rate (mg/L) in water under stirred and unstirred conditions.

TDI ECOTOXICITY

The potential hazards of TDI to aquatic life have been investigated in numerous studies with fish, algae, and invertebrate species. Because TDI is primarily converted to the inert insoluble particles, relatively high concentrations of TDI are required to cause observable lethal or sublethal effects. The conditions associated with these standardized aquatic toxicity tests result in higher degrees of TDI conversion to TDA than would be expected under any plausible emission or spillage scenario. Adverse effects of TDI on aquatic life have been observed primarily with the aquatic invertebrates, and these effects have been directly attributed to the measured amounts of TDA formed under these uncharacteristic conditions of TDI exposure. A selection of aquatic hazard test results for TDI are summarized in Table 2.

Note: Since TDI is not water soluble, aquatic effects are expressed on the basis of nominal loading rates to water, and any observed effects are interpolated from the water-accommodated fractions associated with a series of individually prepared test substance loading rates.

EL₅₀ = Median Effective Loading Rate (causing effects in 50% of exposed population)
 LL₀ = Highest tested loading rate showing no mortality in the exposed population
 LL₅₀ = Median Lethal Loading Rate (causing mortality in 50% of exposed population)
 E_rL₅₀ = Median Effective Loading Rate (causing 50% reduction in growth rate of exposed population)
 NOELR = No Observed Effect Loading Rate (highest loading rate showing no effects of exposed population)
 EC₅₀ = Median Effective Concentration in Soil (dry wt. basis)
 NOEC = No Observed Effect Concentration in Soil (dry wt. basis)

Table 2. Summary of Ecotoxicological Studies Conducted with TDI

Substance	Tested Species	Toxicological Endpoint	Result (mg/L)
80: 20 TDI	Daphnia magna (invertebrate)	48 h EL ₀ 48 h EL ₅₀ (immobilization)	1.6 12.5
80: 20 TDI	Daphnia magna (invertebrate)	48 h EL ₀ 48 h EL ₅₀ (immobilization)	6.25 18.3
80: 20 TDI	Daphnia magna (invertebrate)	21 d EL ₅₀ 21 d NOELR (Reproduction)	2 1.1
80: 20 TDI	Desmodesmus subspicatus (green algae)	96 h ErL ₅₀ 96 h NOELR (growth rate inhibition)	4,300 ≥ 100
80: 20 TDI	Chlorella vulgaris (green algae)	96 h EL ₅₀ (growth)	4,300
80: 20 TDI	Skeletonema costatum (marine diatom)	96 h EL ₅₀ (growth)	3,230
80: 20 TDI	Danio rerio (Zebra fish)	96 h LL ₀ 96 h LL ₅₀ (mortality)	< 100 > 250
80: 20 TDI	Oryzias latipes (Rice fish)	96 h LL ₅₀ (mortality)	4,170
80: 20 TDI	Onchorynchus mykiss (Rainbow trout)	96 h LL ₅₀ (mortality)	133
2, 6-TDI	Pimephales promelas (Fathead Minnow)	96 h LL ₅₀ (mortality)	164
80: 20 TDI	Eisenia fetida (Earthworm)	14 d LC ₅₀ (mortality) 14 d NOEC (biomass) 14 d NOEC (behavior)	> 1,000 mg/kg ≥ 1,000 mg/kg ≥ 1,000 mg/kg
80: 20 TDI	Avena sativa (Oat)	14 d EC ₅₀ (growth rate) 14 d NOEC (emergence) 14 d NOEC (survival) 14 d NOEC growth rate)	> 1,000 mg/kg ≥ 1,000 mg/kg ≥ 1,000 mg/kg ≥ 1,000 mg/kg
80: 20 TDI	Lactuca sativa (Lettuce)	14 d EC ₅₀ (growth rate) 14 d NOEC (emergence) 14 d NOEC (survival) 14 d NOEC growth rate)	> 1,000 mg/kg ≥ 1,000 mg/kg ≥ 1,000 mg/kg ≥ 1,000 mg/kg
80: 20 TDI	Activated Sludge (domestic sewage treatment)	3 h EC ₅₀ (respiration Inhibition)	> 100

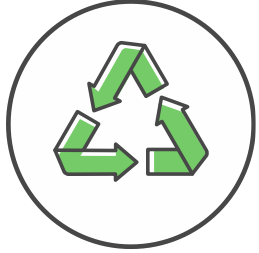
TDI in the Soil Environment

TDI IN THE SOIL AND SEDIMENT

The introduction of TDI to soil, such as could occur during an accidental spillage event, will result in its reaction with water, organic matter, and solid mineral components of the soil. This reactivity will make the liquid TDI immobile in soil, as the spilled material is converted to a mass of combined soil and polyurea solids. The time required for 50% conversion of TDI in soil is expected to be similar to that measured for 4,4-MDI substance, which ranged from about 1 to 7 hours over a wide range of soil types and is a similar reactivity (Holzaht-Grimme, 2018). Polyureas are the predominant reaction product of TDI in soil, and studies have shown these polyureas to be resistant to degradation for millennia (Sendjarevic et al., 2004). If a spill of liquid TDI to soil occurs, it is often recommended to cover the material with wet soil to prevent spread of the material and promote the conversion to polyurea which can be later recovered and disposed as solid waste. As shown in **Table 2**, there are no observed or expected long-term effects of TDI to soil-associated invertebrates and plants.

Any toluenediamine (TDA) which might be formed from hydrolysis of TDI or from degradation of polyurethane materials in the soil environment is expected to be rapidly degraded. Primary aromatic amine substances such as TDA are known to be reacted with the organic matter component of soil and sediment (Cowen et al., 1998). This “chemisorption” of TDA is to a large extent irreversible and serves to reduce the mobility and bioavailability of TDA in soil and sediment compartments. Any TDA which is not consumed in this degradation pathway can be degraded to carbon dioxide and ammonia by microorganisms present in aerobic soils and sediments (Cowen et al., 1998; Boegi et al., 2018)

DISPOSAL – END OF LIFE



RECYCLE/REUSE

A growing variety of options are available for recovery of the material and energy resources associated with TDI-based polyurethane products at the end of their intended service life. Technological advances continue to make possible the integration of polyurethane into the circular economy.



ENERGY RECOVERY

Technology continues to develop which enables re-use and recycling of polyurethane materials derived from TDI. Re-use can involve blending of recovered polyurethane foam with additional diisocyanate binder to make re-bonded polyurethane foam. Thermal- and chemical-based recycling of polyurethane can sometimes result in recovery of the polyol and TDA components which can be repurified or blended with virgin materials to make new polyurethane products.

DISPOSAL – END OF LIFE



DISPOSAL

Laboratory studies have been performed to examine the fate of TDI-based flexible foams under simulated landfill conditions over a two-year period (Brown et al., 1999). The results of this study showed no adverse impacts on landfill decomposition processes (methanogenesis), no visible changes to physical structure of the foams, and a small initial release of TDA from the foam into the recirculating leachate, which eventually dissipated to background levels (~ 2 µg/L). When an aqueous solution of TDA was added to the landfill simulators, only about 5% of it could be initially detected in the recirculating leachate, and the TDA concentration continued to decrease with continued operation and circulation of the landfill simulators. These results indicated that TDA was being efficiently degraded or tightly bound within the simulated landfill components, and if polyurethane degradation can occur within a solid waste landfill, any TDA released as a result has low potential to persist or accumulate in the landfill leachate.



INCINERATION

In some regions and for some types of polyurethane materials, re-use, recycle, and landfill are not available options for disposal or recovery of polyurethane waste material. The various TDI substances and the polyurethane materials derived from them are combustible and are expected to be completely consumed in a municipal solid waste incinerator. Incineration provides a means of energy recovery from polyurethane waste materials which might be difficult to recycle or are otherwise disposed in solid waste landfills. When properly incinerated the products of TDI and polyurethane combustion are indistinguishable from those of other solid waste materials composed on carbon, nitrogen, and oxygen.

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