

# New Chemicals Division’s Approach to Evaluating the Environmental Fate of Mixed Metal Oxides

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## Summary

This memo details the New Chemicals Division (NCD) approach to evaluating the environmental fate of mixed metal oxides (MMOs).

## Background

MMOs are solid compounds that contain two or more different metal cations and the oxide anion ( $O^{2-}$ ). MMOs have many electrical applications in batteries and uses as catalysts, adsorbents, and in ceramics. MMOs are a key component in lithium-ion batteries used in electric vehicles.

NCD has standard ratings for MMOs based on measured data from Premanufacture Notices (PMNs), data from analogous substances, and data from scientific literature, as detailed in this guidance.

In addition to the parent MMO, environmental fate is also assessed for each constituent metal within the MMO. The metals are rated if it is determined that there is a potential for release of the metals from the MMO matrix under environmental conditions. This determination considers the water solubility (measured or estimated) of the MMO and any available leaching/dissolution data for the new chemical substance or an analogous substance. In the absence of applicable data on the new chemical substance or a suitable analogue showing negligible water solubility and leaching, all constituent metals are rated as a conservative approach.

Measured, analogue, and/or estimated data are used to derive ratings for the following fate endpoints:

- Destruction and removal efficiency (DRE)
- Overall removal in wastewater treatment plants (WWTP) and WWTP removal via sorption to sludge, air stripping, and biodegradation
- Environmental biodegradation half-lives (aerobic and anaerobic)
- Abiotic degradation (i.e., hydrolysis, photolysis, and atmospheric oxidation) half-lives
- Sorption to soil and sediment
- Migration to groundwater
- Persistence
- Bioaccumulation potential

Although EPI (Estimation Programs Interface) Suite™ is frequently utilized by NCD, the software is most suitable for estimating the physical-chemical properties and environmental fate behavior of discrete, organic compounds. Inorganic and organometallic compounds, including MMOs and their constituent metals, are not within the domain of applicability for the models. Thus, EPI Suite™ is not used to support MMO or free metal ratings for fate endpoints.

## Ratings and Rationales

The following sections include a summary of the environmental fate ratings and rationales for MMOs.

## Destruction and Removal Efficiency

The destruction and removal efficiency (DRE) is an estimate of the percentage of a given substance entering a hypothetical municipal solid waste incinerator (MSWI) that is anticipated to be removed and/or destroyed by the treatment process. DREs are necessary to estimate stack air releases and other general population exposure scenarios. This rating reflects the anticipated destruction and removal of the chemical by all mechanisms available in a MSWI, including combustion and collection by filter technologies. New chemical substances typically receive either a 0% or 99.9% DRE.

Metal compounds in which there is low pyrolyzable (i.e., organic) content, such as MMOs, will end up captured in fly ash and/or bottom ash following incineration, with a few exceptions, including mercury and selenium.<sup>1,2,3</sup> As such, these releases should be assessed as primarily landfill releases, as opposed to stack air emissions.

A DRE of 99.9% removal to landfill is assigned for MMOs.<sup>4</sup> As a result, 99.9% of the MMO entering the municipal incinerator is assumed to ultimately contribute to the landfill releases and exposures. The remaining 0.1% is accounted for in stack air emissions to address vapor and/or particulate metal releases that cannot be captured by MSWI control technology.

## Overall Removal in Wastewater Treatment Plants

The overall removal of MMOs by WWTPs is estimated to be 90% via very strong sorption to sludge. Removal via stripping and biodegradation are estimated to be negligible. NCD does not assess the WWTP removal of the constituent metals of the MMO, as it is not anticipated that these metals will dissociate from the parent materials in appreciable amounts within the time frame relevant to wastewater treatment processes, which span hours to days.<sup>4</sup>

## WWTP Removal via Sorption to Sludge

NCD typically relies on estimates of the organic carbon to water partition coefficient ( $K_{OC}$ ) to estimate the sorption potential of a new chemical substance. Because EPI Suite™ is not suitable to estimate the physical-chemical and fate properties of MMOs, the  $K_{OC}$  cannot be estimated. Based on their large molecular weight and low water solubility, MMOs are expected to sorb very strongly to sludge in a WWTP.

Literature on the sorption characteristics and WWTP removal of MMOs could not be identified and no measured sorption data associated with MMO cases submitted to NCD were found. Literature available for pure (single-metal) metal oxides supports high removal from wastewater

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<sup>1</sup> Hasselriis, F. and Licata, A., 1996. Analysis of heavy metal emission data from municipal waste combustion. *Journal of hazardous materials*, 47(1-3), pp.77-102.

<sup>2</sup> US EPA. 2025. Energy recovery from the combustion of municipal solid waste (MSW).

<https://www.epa.gov/smm/energy-recovery-combustion-municipal-solid-waste-msw>. Accessed October 20, 2025.

<sup>3</sup> Helble, J.J. 2000. A model for the air emissions of trace metallic elements from coal combustors equipped with electrostatic precipitators. *Fuel Process. Technol.* 63(2-3):125-147.

<sup>4</sup> U.S. EPA, 2025. Revised Procedures for Assessing the Fate and Transport of Mixed Metal Oxides in TSCA New Chemical Assessments, Washington D.C. 2pp.

treatment via sorption to sludge. Particle size significantly influences a chemical's sorption characteristics, with larger molecules sorbing more strongly to sludge, soil, and sediment. Recent MMO submissions to NCD include both nano- and micro-scale substances. Most of the studies identified were carried out on metal oxide nanomaterials, which are analogous to similar sized MMOs for sorption endpoints. Larger (i.e., microscale) MMOs would be predicted to have higher sorption potential than their nanoscale counterparts.

Gottschalk *et al.* (2009) modeled the behavior of titanium dioxide and zinc oxide nanomaterials in the environment and within WWTPs and predicted these substances would partition primarily to sludge, soil, and sediment due to sorption.<sup>5</sup> A study by Limbach *et al.* (2008) that followed the OECD 303A study guideline (Simulation Test - Aerobic Sewage Treatment -- A: Activated Sludge Units) found that cerium oxide nanoparticles were removed at 95–98% in a model WWTP, primarily via sorption to sludge.<sup>6</sup> Qiu *et al.* observed initial removal of >90% titanium dioxide nanoparticles from a sequencing batch reactor via sorption to sludge, though removal dropped to <70% after 60 days due to sorption saturation.<sup>7</sup> Tan *et al.* found that zinc oxide nanoparticles were removed with >95% efficiency in a membrane bioreactor, with 80% of the removal attributed to sorption mechanisms.<sup>8</sup> Finally, Kiser *et al.* measured 91% removal of nano- and micro-scale titanium dioxide via sorption to sludge in a full-scale municipal WWTP.<sup>9</sup>

Based on the studies as well as their large molecular weight and low water solubility, MMOs are assigned a rating of very strong sorption to sludge.

### WWTP Removal via Air Stripping

MMOs are not expected to undergo air stripping during wastewater treatment due to their low vapor pressures, low predicted Henry's law constants, and high molecular weights. Compounds with high molecular weights are hindered from evaporating or volatilizing from the surface of the water. The vapor pressures of MMOs are estimated to be <0.000001 Torr (negligible) which is supported by studies of simple metal oxides that show very low vapor pressures even at extremely high temperatures.<sup>10,11</sup> Henry's law constants cannot be estimated because EPI

<sup>5</sup> Gottschalk, F., Sonderer, T., Scholz, R. W., & Nowack, B. (2009). Modeled environmental concentrations of engineered nanomaterials (TiO<sub>2</sub>, ZnO, Ag, CNT, fullerenes) for different regions. *Environmental science & technology*, 43(24), 9216-9222.

<sup>6</sup> Limbach, L. K., Bereiter, R., Müller, E., Krebs, R., Gälli, R., & Stark, W. J. (2008). Removal of oxide nanoparticles in a model wastewater treatment plant: influence of agglomeration and surfactants on clearing efficiency. *Environmental science & technology*, 42(15), 5828-5833.

<sup>7</sup> Qiu, G., Au, M. J., & Ting, Y. P. (2016). Impacts of nano-TiO<sub>2</sub> on system performance and bacterial community and their removal during biological treatment of wastewater. *Water, Air, & Soil Pollution*, 227, 1-12.

<sup>8</sup> Tan, M., Qiu, G., & Ting, Y. P. (2015). Effects of ZnO nanoparticles on wastewater treatment and their removal behavior in a membrane bioreactor. *Bioresource technology*, 185, 125-133.

<sup>9</sup> Kiser, M. A., Westerhoff, P., Benn, T., Wang, Y., Perez-Rivera, J., & Hristovski, K. (2009). Titanium nanomaterial removal and release from wastewater treatment plants. *Environmental science & technology*, 43(17), 6757-6763.

<sup>10</sup> Schulz, U., Saruhan, B., Fritscher, K., & Leyens, C. (2004). Review on advanced EB-PVD ceramic topcoats for TBC applications. *International journal of applied ceramic technology*, 1(4), 302-315.

<sup>11</sup> Lamoreaux, R. H., Hildenbrand, D. L., & Brewer, L. (1987). High-Temperature Vaporization Behavior of Oxides II. Oxides of Be, Mg, Ca, Sr, Ba, B, Al, Ga, In, Tl, Si, Ge, Sn, Pb, Zn, Cd, and Hg. *Journal of physical and chemical reference data*, 16(3), 419-443.

Suite™ is not suitable for MMOs; however, it can be inferred that the values would be very low based on MMO structure and physical-chemical properties. Thus, MMOs are expected to undergo negligible removal via volatilization in a WWTP. This parameter is not rated for the constituent metals of the MMO.

### WWTP Removal via Biodegradation

MMOs are not expected to undergo biodegradation. Biodegradation, by definition, is the breakdown of organic substances by microorganisms and is not applicable to inorganic compounds, such as MMOs. Consequently, negligible removal of MMOs is expected via biodegradation in a WWTP. This parameter is not rated for the constituent metals of the MMO.

### Environmental Biodegradation

Neither MMOs nor their constituent metals are expected to undergo biodegradation under environmental conditions. Biodegradation, by definition, is the breakdown of organic substances by microorganisms and is not applicable to inorganic compounds, such as MMOs and metals. A biodegradation half-life of > 6 months is expected for MMOs and their constituent metals in both aerobic (e.g., surface water) and anaerobic (e.g., sediment) environments.

### Hydrolysis

MMOs are not expected to undergo hydrolysis. These substances do not have functional groups that would enable them to undergo hydrolysis. The constituent metals themselves cannot be hydrolyzed but may participate in hydrolysis reactions by acting as Lewis acids in water, which may ultimately lead to the formation of metal oxides or hydroxides.<sup>12</sup> Modeling these reactions is complex and beyond the scope of NCD's screening level assessments. The hydrolysis potential of MMOs and their constituent metals is not assessed, and hydrolysis half-lives are not assigned.

### Photolysis

MMOs and their constituent metals do not contain chromophores. Photolysis is not expected. Metals can play a role as a catalyst in the photolysis of other compounds, but this is outside the scope of a new chemical environmental fate assessment.<sup>13,14</sup> Therefore, the photolysis potential of MMOs and their constituent metals is not evaluated, and photolysis half-lives are not assigned.

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<sup>12</sup> Corma, A., & García, H. (2002). Lewis acids as catalysts in oxidation reactions: from homogeneous to heterogeneous systems. *Chemical Reviews*, 102(10), 3837-3892.

<sup>13</sup> Prier, C. K., Rankic, D. A., & MacMillan, D. W. (2013). Visible light photoredox catalysis with transition metal complexes: applications in organic synthesis. *Chemical reviews*, 113(7), 5322-5363.

<sup>14</sup> Koppenol, W. H. (1993). The centennial of the Fenton reaction. *Free Radical Biology and Medicine*, 15(6), 645-651.

## Atmospheric Oxidation

MMOs are not expected to undergo atmospheric oxidation. The compounds are not volatile, already exist in their oxidized state, and are thus not expected to react with hydroxyl radicals or ozone. Free metals may undergo atmospheric oxidation to form metal oxides.<sup>15</sup> Modeling these reactions is complex and beyond the scope of NCD's screening level assessments. Therefore, the atmospheric oxidation potential of MMOs and their constituent metals is not assessed, and oxidation half-lives are not assigned.

## Sorption to Soil and Sediment

NCD typically relies on K<sub>oc</sub> estimates to estimate the sorption potential of new chemical substances. Because EPI Suite™ is not suitable to estimate the physical-chemical and fate properties of MMOs, a K<sub>OC</sub> cannot be estimated for these substances. Based on their large molecular weight and low water solubility, MMOs are expected to sorb strongly to soil and sediment.

As mentioned previously, metal oxide nanomaterials are considered analogues to MMOs for sorption endpoints. Gottschalk *et al.* (2009) modeled the behavior of titanium dioxide and zinc oxide nanomaterials in the environment and within WWTPs and predicted these substances would partition primarily to sludge, soil, and sediment due to sorption.<sup>5</sup> Based on the study as well as their large molecular weight and low water solubility, MMOs are assigned a rating of very strong sorption to soil and sediment.

Individual metals have a wide range of sorptive efficiencies. The sorption to soil and sediment rating for constituent metals is based on available scientific literature for each metal. Thus, the sorption to soil and sediment rating is unique to each metal assessed.

## Migration to Groundwater

The migration to groundwater ratings for MMOs and their constituent metals are based on the respective sorption to soil and sediment rating, according to the NCD Environmental Fate Assessment Process Overview and Rating Guidance.<sup>16</sup> There are no mitigating factors (e.g., biodegradation or hydrolysis).

MMOs are expected to have low potential to migrate to groundwater. Negligible migration is expected based on very strong sorption to soil and sediment. The groundwater migration potential for the constituent metals will be unique to each metal and based on the metal's sorption to soil and sediment rating.

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<sup>15</sup> Cabrera, N. F. M. N., & Mott, N. F. (1949). Theory of the oxidation of metals. Reports on progress in physics, 12(1), 163.

<sup>16</sup> EPA (2024). New Chemicals Division: Environmental Fate Assessment Process Overview and Rating Guidance. SOP No. NCD-PRG-FATE- 23-0001. May 27, 2024. 35pp.

### Persistence: P Rating

The environmental half-lives of MMOs and metals are expected to be greater than six months in aerobic environments (e.g., surface water) and anaerobic environments (e.g., sediment) based on lack of degradation by biodegradation, hydrolysis, or atmospheric oxidation. Based on NCD's PBT Policy and the NCD Environmental Fate Assessment Process Overview and Rating Guidance, this half-life corresponds to a chemical being considered very persistent.<sup>16,17</sup> MMOs and their constituent metals are therefore assigned a persistence rating of P3 (very persistent).

### Bioaccumulation: B Rating

As inorganic substances, MMOs and their constituent metals are not expected to bioaccumulate via lipophilic partitioning. These substances are rated B\*low or B\*high. "B\*" denotes that the rating is for a chemical that does not bioaccumulate via lipophilic partitioning. The "low" or "high" designation indicates whether the chemical is expected to have low or high potential to bioaccumulate via other mechanisms.

Chemicals with molecular weights  $\geq 1,000$  and/or cross-sectional diameters  $\geq 20 \text{ \AA}$  (2 nm or 0.002  $\mu\text{m}$ ) are typically not bioaccumulative.<sup>16</sup> Consequently, MMOs are not expected to bioaccumulate based on their large molecular weight, molecular volume, and particle size. They are therefore assigned a bioaccumulation rating of B\*low, indicating they do not bioaccumulate via lipophilic partitioning and are not expected to bioaccumulate via other mechanisms based on their large molecular volume.

The bioaccumulation potential of the constituent metals is rated according to the NCD Environmental Fate Assessment Process Overview and Rating Guidance and the New Approach for Evaluating the Bioaccumulation Potential of Metals in the New Chemicals Division.<sup>16,18</sup> A weight of evidence approach, which integrates multiple lines of evidence to assign a rating of B\*low (low bioaccumulation potential) or B\*high (high bioaccumulation potential) to each metal, is employed. Individual, metal-specific bioaccumulation assessments are detailed in reports that are attached to MMO fate assessment reports. The constituent metals are therefore rated B\*low or B\* high, depending on the identity and properties of the specific metal, based on the findings of the weight of evidence approach.

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<sup>17</sup> EPA (2024). Points to Consider When Preparing TSCA New Chemical Notifications. [https://www.epa.gov/sites/default/files/2018-06/documents/points\\_to\\_consider\\_document\\_2018-06-19\\_resp\\_to\\_omb.pdf](https://www.epa.gov/sites/default/files/2018-06/documents/points_to_consider_document_2018-06-19_resp_to_omb.pdf)

<sup>18</sup> U.S. EPA, Office of Pollution Prevention and Toxics, New Chemicals Division. New Approach for Evaluating the Bioaccumulation Potential of Metals in the New Chemicals Division. January 13, 2025. [https://www.epa.gov/system/files/documents/2025-01/ncd\\_metal\\_bioaccumulation-approach\\_final\\_13jan2025\\_ncd-ref-library.pdf](https://www.epa.gov/system/files/documents/2025-01/ncd_metal_bioaccumulation-approach_final_13jan2025_ncd-ref-library.pdf)

### Summary of Fate Ratings for MMOs

Parameters	Ratings for MMOs	Ratings for Constituent Metals
DRE	99.9% removal to landfill	Not rated
Overall Removal in WWTP	90%	Not rated
Removal via adsorption	Very strong	Not rated
Removal via volatilization	Negligible	Not rated
Removal via biodegradation	Negligible	Not rated
Aerobic Biodegradation Half-life	> 6 months	> 6 months
Anaerobic Biodegradation Half-life	> 6 months	> 6 months
Hydrolysis Half-life	Not rated.	Not rated.
Photolysis Half-life	Not rated.	Not rated.
Atmospheric Oxidation Half-life	Not rated.	Not rated.
Sorption to soil and sediment	Very strong	Low to very strong, depending on identity of the metal
Migration to groundwater	Negligible	Negligible to rapid, depending on identity of the metal
Persistence Call	P3	P3
Bioaccumulation Call	B*low	B*low or B*high, depending on identity of the metal

### Fate Testing Recommendations for MMOs

No OECD testing is recommended for the rating of the parent MMOs' environmental fate parameters. EPA believes that the information and data presented in this guidance fulfills all endpoints for MMOs. To refine the assessment of free metals, EPA recommends water solubility (e.g., OECD 105) or dissolution (e.g., OECD 29) data to inform whether constituent metals may be released from parent MMOs in the environment.<sup>19,20</sup>

<sup>19</sup> OECD (1995), Test No. 105: Water Solubility, OECD Guidelines for the Testing of Chemicals, Section 1, OECD Publishing, Paris, <https://doi.org/10.1787/9789264069589-en>.

<sup>20</sup> OECD (2002), Guidance Document on Transformation/Dissolution of Metals and Metal Compounds in Aqueous Media, OECD Series on Testing and Assessment, No. 29, OECD Publishing, Paris, <https://doi.org/10.1787/9789264078451-en>.