# Experiencing REACH Exposure Assessments

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# Exposure Assessments under REACH

**Outline**

1) **Okay – so you know you need a quantitative exposure assessment for a substance, what do you do now?**
2) **Must gather Use information for substance**
3) **Develop an Exposure Scenario for each relevant use**
4) **Tier 1 Exposure Assessment & Risk Characterization (assumes limited knowledge with conservative inputs)**
5) **Tier 2 Exposure Assessment & Risk Characterization (gather more detailed information for input into Tier 2 models)**
6) **So what did we learn?**
7) **Useful References**

# How do we assess exposure quantitatively under REACH?

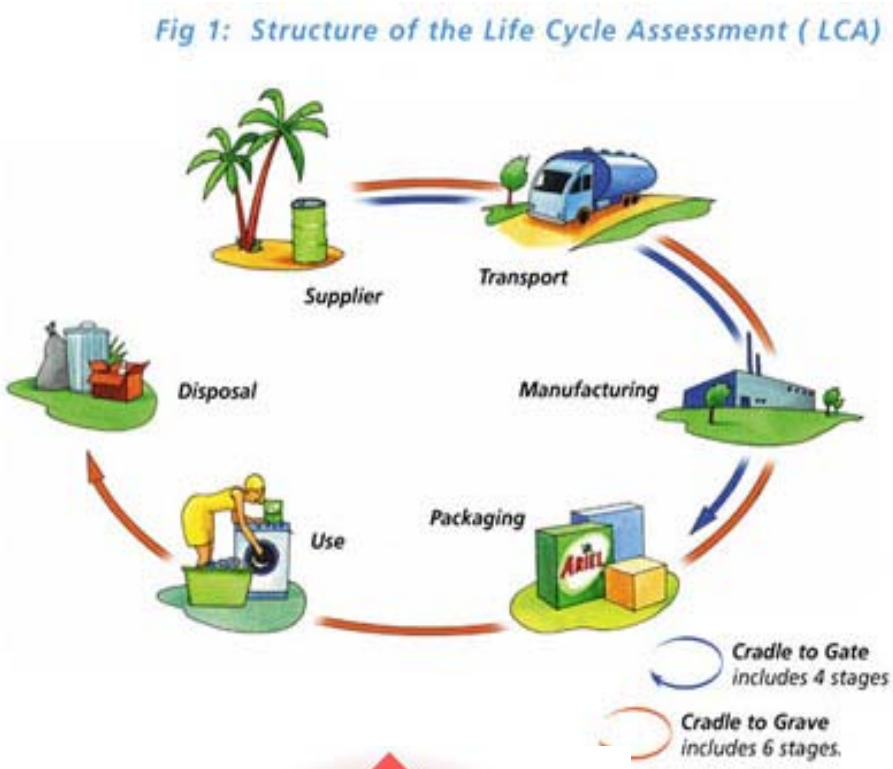
## 1) Identify uses of chemical

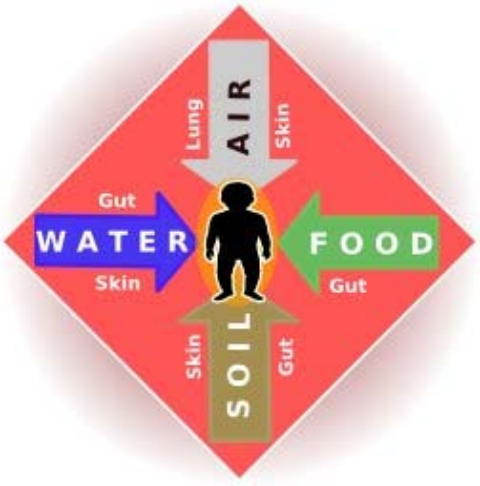
Manufacturing, industrial use, service life, waste

## 2) Identify routes of potential exposure for each use

- Human Exposure: -worker, professional, consumer
- Environmental Exposure:
  - industrial (local, not dispersive),
  - Consumer/professional (regional, wide dispersive)
  - Releases to air, water, soil

## 3) Develop Exposure Scenario for each use



# Develop Exposure Scenario – Worker

**Tier 1 (most conservative)**

**Inputs for Model**

- **Select use descriptors (PROCs) based on type of activity**
- **Time of activity**
- **% of substance used**
- **Form of substance (gas, liquid, solid)**
- **Vapor pressure, dustiness**
- **Operational temperatures**
- **Location of activity: indoors, outdoors, local exhaust ventilation –Y/N**
- **Risk Management Measures (none)**

| PROCs | Description |
|---|---|
| 1 | Use in closed process, no likelihood of exposure |
| 2 | Use in closed, continuous process with occasional controlled exposure |
| 4 | Use in batch and other process (synthesis) where opportunity for exposure arises |
| 5 | Mixing or blending in batch processes (significant contact) |
| 7 | Industrial spraying |
| 8 | Transfer of chemicals from/to vessels/ large containers |
| 9 | Transfer of chemicals into small containers (dedicated filling line) |
| 10 | Roller application or brushing |
| 14 | Production of preparations or articles by tabletting, compression, extrusion, |
| 15 | Use of laboratory reagents in small scale laboratories |

# Run the Tier 1 Model (ECETOC-TRAM)

## Worker Exposure Estimates for a methanol example

| Scenario name | PROC | Type of setting | Is substance a solid? | Duration of activity [hours/day] | Use of ventilation | Inhalative Exposure Estimate (mg/m3) | Dermal Exposure Estimate (mg/kg/day) |
|---|---|---|---|---|---|---|---|
| Generic processing closed systems (liquid) | PROC 2 | industrial | No | >4 hours (default) | Indoors without LEV | 66.8 | 1.4 |
| loading/unloading dedicated facility | PROC 8a | industrial | No | >4 hours (default) | Indoors without LEV | 333.8 | 13.7 |
| mixing and blending | PROC 5 | industrial | No | >4 hours (default) | Indoors without LEV | 333.8 | 13.7 |
| transfer to smaller containers dedicated fill line | PROC 9 | industrial | No | >4 hours (default) | Indoors without LEV | 267.0 | 6.9 |

**Now would compare results to health benchmarks (DNELs)**

**Fails old benchmarks such as ACGIH 8 hr TWA of 260 mg/m3**
**IRIS RfD = 0.5 mg/kg/day indicates dermal could be a problem too**

**As in many of the Tier 1 estimates the risk characterization indicates there is not control of risk so refinement is needed**

# Develop Exposure Scenario – Consumer

**<u>Tier 1 (most conservative)</u>**
**Inputs for Model**

- **Select Sentenial Product (PC/AC)**
- **Select sub product category**
- **Time of activity/day**
- **Amount of product used per use**
- **% substance in product**

**Model has preselected the route of exposure (inhalation, dermal, oral) and has conservative estimates**

| | |
|---|---|
| **PC9a_Coatings_paints_thinners_removers** | Waterborne latex wall paint |
| | Solvent rich, high solid, water borne paint |
| | Aerosol spray can |
| | Removers (paint-, glue-, wall paper-, sealant-remover) |

**Sentenial Product List**

| |
|---|
| **PC1_Adhesives_sealants** |
| **PC3_Air_care_products** |
| **PC9a_Coatings_paints_thinners_removers** |
| **PC9b_Fillers_putties_plasters_modelling_clay** |
| **PC9c_Finger_paints** |
| **PC12_Fertilizers** |
| **PC13_Fuels** |
| **PC24_Lubricants_greases_and_release_products** |
| **PC31_Polishes_and_wax_blends** |
| **PC35_Washing_and_cleaning_products_including_solvent_based_products** |
| **AC5_Fabrics_textiles_and_apparel** |
| **AC6_Leather_articles** |
| **AC8_Paper_articles** |
| **AC10_Rubber_articles** |
| **AC11_Wood_articles** |
| **AC13_Plastic_articles** |

# Run Tier 1 Model for Consumer Use

## Inhalation

**Note: no averaging for days exposure**

The TRA calculates the inhalation exposure as

- concentration in room air (mg/m3) over a day, resulting from one or more events of product/article application.

Or as

- dose (amount per kg bodyweight) inhaled over the duration of the event (depending on the product category 20 min to 8h).

**Concentration:**

| Parameter: | Product Ingredient (g/g) | Amount Product Used per Application (g/event) | Frequency of Use (events / day) | Fraction Released to Air (g/g) | Conversion Factor | Room Volume ($m^3$) | Exposure Air concentration mg/m3 |
|---|---|---|---|---|---|---|---|
| **Algorithm:** | **(PI x** | **A x** | **FQ x** | **F x** | **1000)** | **/ V** | **$C_{inh}$** |

**Dose:**

| Para-meter: | Product Ingred. (g/g) | Amount Product Used per Application (g/event) | Frequency of Use (events / day) | Fraction Released to Air (g/g) | Exposure Time (hr) | Inhalation Rate ($m^3$/hr) | Conversion Factor | Room Volume ($m^3$) | Body Weight (kg) | Exposure Inhalatory dose mg/kg/ day |
|---|---|---|---|---|---|---|---|---|---|---|
| **Algo-rithm:** | **(PI x** | **A x** | **FQ x** | **F x** | **ET x** | **IR x** | **1000)** | **/ (V x** | **BW)** | **$D_{inh}$** |

**FQ: Assumes 100 % available for Vp > 10 Pa, reductions for less volatile**

# Run Tier 1 Model for Consumer Use

***For dermal route:***

| Parameter: | Product Ingredient (g/g) | Contact Area ($cm^2$) | Frequency of use (events / day) | Thickness of Layer (cm) | Density ($g/cm^3$) | Conversion Factor (mg/g) | Body Weight (kg) | Exposure Dermal dose (mg/kg/day) |
|---|---|---|---|---|---|---|---|---|
| **Algorithm:** | **(PI x** | **CA x** | **FQ x** | **TL x** | **D x** | **1000)** | **/ BW** | **$D_{der}$** |

The algorithm for the calculation of the dermal dose does not take into account any duration factor and assumes 100% transfer of substance from the product or article contact layer (0.01 and 0.001 cm respectively) to the skin instantaneously. The dermal absorption is set at 100 %.

***For oral route:***

| Parameter: | Product Ingredient (g/g) | Volume of product swallowed ($cm^3$) | Frequency of use (events / day) | Density (g/cm3) | Conversion Factor (mg/g) | Body Weight (kg) | Exposure Oral dose (mg/kg/day) |
|---|---|---|---|---|---|---|---|
| **Algorithm:** | **(PI x** | **V x** | **FQ x** | **D x** | **1000)** | **/ BW** | **$D_{oral}$** |

**Calculations are very conservative**

# Refinements (Tier 2)

## Human Exposure Refinement

- **Add in Risk Management Measures such as PPE**
  - Respiratory Protective Equipment (RPE) – this area is reasonably defined. In both EU and US similar assigned protection factors (APF) are used. E.g. Full face mask with cartridge filters offers a APF = 20 or a 99.5% efficiency.
  - Chemical Protective gloves – use a glove that offers chemical resistance to substance. Protection factors have been based on level of training and supervision. Typical APF = 10 and includes proper training in using the glove.
  - If substance is volatile, an equation can be used to estimate the evaporation from the skin since substance would evaporate and reduce dermal exposure. (see R14 guidance)
- **Use a Tier 2 model**
  - For REACH there is ART, Consexpo, Stoffenmanager, RISKOFDERM.
  - Unfortunately now much more information is needed:
    - Location/Facility: indoors, outdoors, size of room, air exchanges per hour
    - Amount of substance used (large quantities to small)
    - Have to choose activities with more detail (amount of substance handled per unit time, near far field exposures)
    - More detail on the local exhaust ventilation systems (hoods, vapor recovery systems)
    - Dermal absorption information

# Example of Consumer use of propellant sprays

**Substance very volatile, inhalation main route of exposure.**

**Worst case spray can is 50% propellant, 10 grams product/use**

## Tier 1 Model Inputs

| Descriptor | Product Subcategory | Product Ingredient (g/g) | Amount of prod for formula (g/event) | Exposure Time (hr) | FreQ of Use (events/day) |
|---|---|---|---|---|---|
| PC3_Air_care_products | Aircare, instant action (aerosol sprays) | 0.5 | 10 | 0.25 | 4 |
| PC24_Lubricants_greases_and_release_products | Sprays (based on aerosol spray can) | 0.5 | 300 | 4 | 1 |

## Comparison of 3 models

| Consumer Use | Inhalation exposure ($mg/m^3$) | Inhalation exposure ($mg/kg_{bw}/d$) |
|---|---|---|
| TRAM PC3 (aerosol) | 1.00E+03[a] | 5.71E+00 |
| TRAM PC9a (spray can) | 7.50E+03[a] | **5.71E+01** |
| AISE FURNITURE, FLOOR & LEATHER CARE AISE C20, PC31 | -- | 8.01E-01 |
| AISE SURFACE CLEANERS (AISE C7, PC35) | -- | 6.01E-01 |
| AISE AIR FRESHENERS AEROSOL (AISE C17, PC3) | -- | 2.98E+00 |
| ConsExpo spray paint can model | 1.50E+02 | 5.00E+01[b] |
| ConsExpo disinfectant spray | 1.68E-01 | 5.60E-02[b] |
| ConsExpo hairspray use | 4.82E-01 | 1.61E-01[b] |

[a] ECETOC TRA consumer inhalation exposure is a single event concentration and does not account for room volume dilution so is a very conservative exposure estimate.

[b] Converted from $mg/m^3$ using adult BW of 60 kg of inhalation rate of 20 $m^3$/day. ConsExpo also provides a mean concentration on day of exposure, which would be lower than the mean event dose. Using the mean event dose provides more conservative exposure estimates.

# Develop Exposure Scenario – Environmental

**Tier 1 (most conservative)**

- **Tonnage/yr for each use**
- **Days of use/yr (20, 365)**
- **Vapor Pressure**
- **Water solubility**
- **Log Kow (Partition coefficient)**
- **Biodegradability**
- **Koc or associated QSAR Class**
- **Environmental release criteria (ERCs)**
  - Extremely conservative release estimates
- **Sewage Treatment Plant (STP): Y/N**

| ERC | Description | Release to air | Release to water |
|---|---|---|---|
| ERC1 | Production of chemicals | 5% | 6% |
| ERC2 | Formulation of preparations | 2.50% | 2% |
| ERC4 | Industrial use of processing aids | 100% | 100% |
| ERC5 | Industrial use resulting in inclusion into a matrix | 50% | 50% |
| ERC6c | Production of plastics | 5% | 5% |
| ERC8a | Wide dispersive indoor use of processing aids in open systems | 100% | 100% |
| ERC8c | Wide dispersive indoor use resulting in inclusion into a matrix | 15% | 1% |
| ERC10a | Wide dispersive outdoor use of long-life articles and materials with low release | 0.05% | 3.2% |
| ERC10b | Wide dispersive outdoor use of long-life articles with intended release | 100% | 100% |

# Run the Tier 1 Model (ECETOC-TRAM)

## Environmental Exposure Estimates

**The ECETOC-TRAM model is based on the EUSES environmental model. Designed to be conservative. Based on the physio-chemical properties, substance is distributed in the various environmental compartments. Key input is releases to environment (kg/day).**

**Example: a non volatile monomer is polymerized at a site, very water soluble, not biodegradable, 2000 tonnes, ERC6c (5% release to air and water)**

| Risk Chacteristation Ratio for Environmental Compartments | Must be <1 |
|---|---|
| RCR STP | 25 |
| RCR freshwater | 2500 |
| RCR sediment | 2500 |
| RCR terrestial | 0.4 |

**Again results need a great deal of refinement to achieve control of risk. Fortunately, effluent is monitored so have data to refine releases. Final releases were <20 g/day versus 50 kg/day for Tier 1 default.**

# Refinements (Tier 2)

## Environmental Exposure Refinement

- The key is to refine the releases since they are the main driver for the predicted environmental concentrations.
- OECD documents on emissions are useful
- Use actual emissions from industrial sites if known

- Industry Work groups develop emission refinements
  - Various industry groups in the EU got together and developed generic emissions that better represent their industrial uses than the ERCs. These are now included in the TRAM model for refinement options. This was a great improvement.
- TRAM model uses a standard 1/10 dilution for STP effluent into river water. Having actual STP flows and river flows allows for higher dilutions.
- Usually manage to refine within the TRAM model.
- Tier 2 models are available but require extensive inputs
  - GEMCO for estuary and marine environments. Was used successfully but need specific inputs.

# So what have we learned?

•It is a complex effort to estimate exposures and requires a variety of information early on in the process.

•Need to compile use information for your company and any downstream users. Complicated to ask for all the Tier 2 information so typically start with Tier 1. Need a standardized language to communicate with (i.e. PROCs and ERCs for EU).

•Need final physical chemical data points and hazard classification early in the process or there will be rework.

•It was harder than we expected since Tier 1 approaches seldom produced risk characterizations below 1. It can take ~200 hrs to gather info, perform and document a Tier 2 exposure assessment for a substance with 3 uses.

•Need to develop generic scenarios that cover multiple uses if possible to reduce the overall work load.

# References

- The Final ECHA Guidance on information requirements and safety assessment documents R14, 15, 16 are worth reading for exposure assessment information
- R14: Occupational Exposure Estimation (May 2010) gives references and discussions on the models
- R15: Consumer Exposure Estimation (April 2010) gives references and discussions on the models
- R16: Environmental Exposure Estimation (May 2010), extensive information on the calculations for TRAM model (based on EUSES)
- http://guidance.echa.europa.eu/docs/guidance_document/information_requirements_en.htm#r14 (one website has links to all the REACH guidance documents, scroll down to bottom to find R14-16)
- ECETOC TRAM Model (Tier 1 tool for REACH) download at http://www.ecetoc.org/index.php?page=tra
- AISE model website (Association International of Soaps and Detergents) http://www.aise.eu/reach/exposureass_sub3.htm
- Consexpo 4.1 Model download at http://www.rivm.nl/en/healthanddisease/productsafety/Main.jsp
- Stoffenmanager Model website https://www.stoffenmanager.nl/Default.aspx (hit the English button, have to request a password)
- ART (Advanced REACH Tool) Model: http://xnet.hsl.gov.uk/art/ (have to request a password)

# Questions?

Thank you

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