REACH Waste Life Stage Emission Calculator

Organic Chemicals, Solvents

Background Document

1.   Introduction and Scope

The calculator tool is designed to provide a substance manufacturer / importer in the organic chemicals / solvents sector with a method of estimating a release of a particular substance resulting from its waste life stage, a requirement resulting from REACH legislation.

It is limited in scope to estimating a substance's release to atmosphere as the main release route; it does not consider other releases, such as those from combustion products etc.

Thus it provides for a coherent and consistent methodology for both producers or importers to calculate air path emissions. This is the first version of this a tool and it will undoubtedly evolve in future versions. It includes within its scope the main recovery/disposal options available for waste (liquid) organic chemicals / solvents currently used in Europe, namely:

- Solvent Recovery by Distillation
- Energy Recovery as a Secondary (Liquid) Fuel in the Cement & Lime Industry
- Disposal by Incineration

This methodology has been put together with cooperation from leading European waste recycling / recovery companies. The help of the following trade bodies is gratefully acknowledged :

- German Association of Chemical Trade and Distribution (Verband Chemiehandel)
- British Chemical Recycling Association (CRA), UK

- CEFIC
- Chemical Industries Association (CIA), UK
- European Cement (Industry) Association (Cembureau)
- British Cement Association, UK

2. Methodology

2.1 Solvent Recovery by Distillation

For the purpose of the release estimation, a conceptual model of a solvent recovery process is used. Input waste crude material is offloaded into a storage tank which vents to atmosphere via any one of a variety of VOC abatement technologies. Such inputs may be pre-processed prior to distillation.

Following the main distillation stage and condensation, through any number of condenser technologies to deliver a recycled product, the residual emissions are sent to an abatement plant before finally being released to atmosphere. Other wastes from the process include distillation residues and process effluents; these however are excluded from the scope of this air emission release calculator.

This methodology ahs been developed on the basis of a number of assumptions relating to process steps and efficiencies that are typical of the Best Available Technique approach adopted under the IPPC Directive. This method thus substitutes for industry site specific emission limits which are not consistently available.
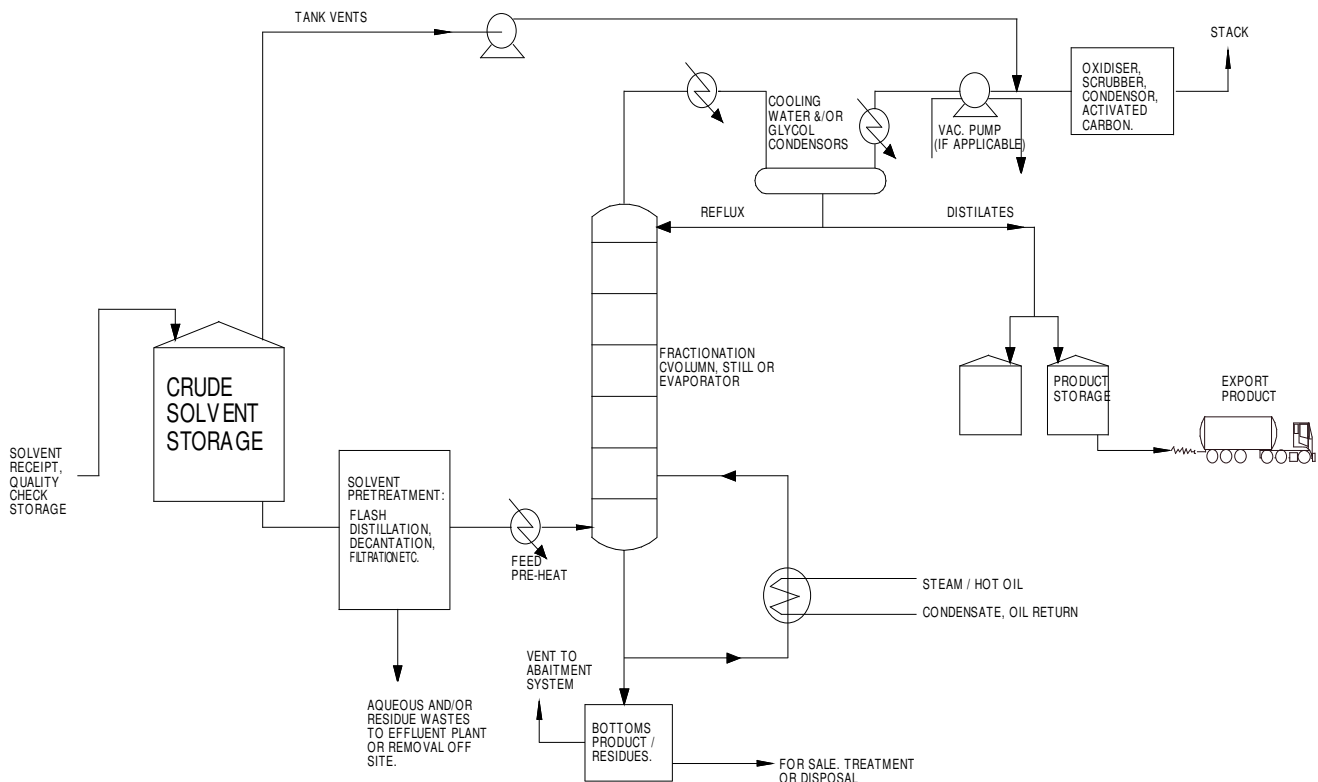
Releases from Storage Tanks

The maximum estimated releases quantified in this calculator are derived via determinations of vapour pressure (from first principles - via the use of Antoine Coefficients) of the substance at a given temperature. It then assumes that the volume of air equivalent to the liquid volume input into a tank is released as a displacement process. It is further assumed that the material will be filled into two separate tanks (crude and product). Abatement of releases is taken into account via a user inputted choice of abatement technique and its assumed /related efficiency.

USER INPUT: the user inputs certain physical properties of the substance and an average annual ambient temperature for the relevant region / country. Abatement efficiency is estimated from guidance tables available for most abatement techniques.

CALCULATION STAGES: the tool calculates the maximum concentration of the substance in air, assuming no time-constraint of the rate of evaporation of the substance in the tank. It is assumed that the head-space of the tank is completely saturated with the maximum concentration of a substance ("equilibrium concentration") it can hold. The volume of substance in the tank is then calculated using input specific gravity data.

It is further assumed that once the relevant volume of substance has been transferred from the tank, the tank would be re-filled by that same amount and that the subsequent air displaced equates to the volume release of substance to a downstream abatement process. This calculation stage is performed twice on the basis that notionally one tank filling step would be required for the crude waste input and a second storage tank filling operation would be required for the processed, recovered product.

The volume release for the product storage phase allows for the previous losses from crude storage and the distillation process itself (and is therefore always slightly less than the release from the crude waste input storage). The user input abatement efficiency tool (allows 0 – 3 abatement efficiencies to be inputted); it then applies an accepted industry average abatement efficiency to this release to finally calculate an actual release to atmosphere from crude storage and from product storage. The tool is pre-selected for a typical plant that has certain (in this case product-specific scrubbing) capabilities for storage tank releases.

Release from distillation condensers

It is assumed that all the substance is evaporated during the distillation process and that the process release (prior to any pollution control abatement plant) is limited only by the efficiency of the condensing equipment. Although it will always be the aim of the recycler to maximise condenser efficiency, for these purposes this calculation will in effect provide a maximum release estimate. The User Input can input 1 or 2 condensing stages before selecting between 0 and 3 abatement options. Once provided with the assumed or actual plant operating parameters/ set-up, the tool calculates the total mass release of substance to the environment. The tool is pre-selected for a typical/ average plant that has a single condenser stage followed by a gas washing "scrubber" and off-gas incineration process.

Pre-set example

The data in the green fields is pre-entered using **ethanol** as an example. The green fields must be over-written by the USER with site/substance specific input requirements.

2.2   Co-Incineration in Cement / Lime Kilns and Incineration Processes

For the purpose of estimating releases from co-incineration and incineration plant, only substance emissions to atmosphere from incomplete combustion processes are considered. These emissions are calculated as the theoretical maximum case emissions based on the emission limit value for total organic carbon stipulated in the Waste Incineration Directive. Storage related emissions are not considered.

USER input: the user inputs the chemical composition and some physical parameters of the substance. The example spreadsheet is pre-completed for **toluene.** The relevant emission limit and reference condition that apply are also user defined (section 2), though these are pre-completed using conditions from the Waste Incineration Directive. Finally, the user specifies the unit of measure to be used (weight or volume) in section 3.

The calculator tool then uses the user input data to derive emission estimations for both co-incineration and incineration processes in the following four stage manner.

Firstly, in order to relate the emission limit value (which is expressed as a concentration to a mass input of waste) the volume of gas and air resulting from the combustion process has to be determined. The calculator assumes complete combustion (e.g. all carbon to carbon dioxide etc). It then applies the Ideal Gas Equation to determine the volume of combustion gas released directly from the combustion process. Note that hydrogen in the waste is assumed to form water and as the reference conditions for emission limit values are referenced to a dry gas, water / steam is then subsequently discounted.

Secondly, the tool determines the amount of oxygen required to support this combustion and at a user-defined oxygen concentration in air (pre-set at 20.9%) it determines the volume of completely oxygen depleted air left in the post-combustion gas stream.

Thirdly, the tool determines the volume of excess air to provide the previously stipulated oxygen reference condition in the off-gas.

By addition of these gas / air volumes and applying the Waste Incineration Directive emission limit for Total Organic Carbon entirely to the substance in question, the theoretical maximum substance emission, normalised as carbon, is determined.

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