Guide to calculation worksheets

I. Overview

I.A. Purpose and domain of this tool

This tool intends to facilitate the calculation of *direct* CO₂ emissions from the production of ammonia (NH₃). This document is to be used in conjunction with two additional documents:

 'Calculation worksheets – Calculating CO₂ emissions from the production of ammonia (NH₃)' (Version 2.0), and

• 'GHG Protocol Reporting Standard and Guidance'.

A step-by-step approach is used to cover every phase of the calculation process from data gathering to reporting.

This is a sector-specific tool, which should be applied by all companies whose operations involve the production of ammonia (NH₃).

I.B. Estimation method used in the tool

In general there are two estimation methodologies that can be used to calculate a company's GHG emissions:

- emission factor based methodology
- direct monitoring

Both are acceptable ways to estimate GHG emissions. Usually companies will use the emission factor based methodology. The direct monitoring approach is more commonly used to measure non-CO₂ process emissions. If a direct monitoring system has already been established in a facility, the associated data provides a good estimate of CO₂ emissions.

This tool is based on the emission factor based methodology, which multiplies activity data (the amount of ammonia produced by a plant) by an emission factor that describes the amount of energy required to produce one tonne of ammonia. The resulting estimate of energy consumption is combined with carbon content data to calculate the CO_2 emissions arising from a plant's ammonia production.

I.C. Process description

Anhydrous ammonia is synthesized by reacting hydrogen with nitrogen at a molar ratio of 3 to 1. Nitrogen is obtained from the air through liquid air distillation or an oxidative process where air is burnt and the residual nitrogen is recovered. Most hydrogen is obtained from natural gas (chiefly methane (CH₄)), although it can also be obtained from other hydrocarbons, such as oil and coal, or water. The carbon content of the hydrocarbon is eliminated from the ammonia synthesis process at several stages (primary steam reforming and shift conversion stages) through conversion to carbon dioxide (CO₂). This CO₂ is the main potential direct greenhouse gas emission, although additional sources of CO₂ emissions include regeneration of the CO₂ scrubbing solution used to capture CO₂ as well as condensate stripping. The actual or realized emissions of CO₂ are determined by the extent of carbon storage and sequestration (CSS) technologies and of urea synthesis.

Please note that in ammonia production no distinction is made between emissions from the stationary combustion of fuel and emissions from feedstock use. This is because fuels typically serve dual energy and process uses in the ammonia sector.

I.D. Assumptions

This guideline is built on the assumption that all carbon contained in the feedstock used for ammonia production is emitted to the air in the form of CO₂ (EPA, 1993).

II. Choice of emission factors

The preferred approach is to use customized emission factors. Customized factors might be available from the suppliers of the technology used to synthesize ammonia. They can also be calculated by individual plants should a plant have access to time series data on the amount of energy used to produce ammonia and on the production output. If customized factors are used, clearly state this in the final report and explain how customized factors have been derived. This tool also provides a wide range of typical emission factors that enable users calculate to CO₂ emissions in a time-efficient manner. However, these typical factors only represent an estimation of fuel properties. Also, please note that the default factors pertain only to natural gas (specifically methane) as natural gas is the feedstock predominantly used by ammonia plants.

III. Emissions calculation

To calculate direct CO_2 emissions, you need to determine the quantity of ammonia produced, an appropriate emissions factor, the fraction of the feedstock's carbon that was oxidized during ammonia synthesis, and the amount of CO_2 that was sequestered by CSS technologies or for urea synthesis.

The following steps are required to be undertaken to calculate the CO₂ emissions using the Excel workbook:

- 1. Enter the production process used by the reporting plant in Column A.
- 2. Enter the quantity of ammonia (in metric tonnes) produced in column B. To increase transparency, it is recommended to enter data separately for each source and fuel type; in other words, where possible companies should disaggregate their production data both by the production process and by the feedstocks used.
- 3. Enter the fuel-specific and process-specific emission factor in column D. A list of typical emission factors can be found in the 'Method' tab of the Excel workbook, although it is always recommended to use custom emission factors to achieve better accuracy of data. The emission factor should be compatible with the fuel use data input; i.e., it should be expressed in the same units the production data were expressed in.
- 4. Enter an appropriate carbon content factor in Column E and an appropriate carbon oxidation factor in Column F. These values should be fuel-specific, and fuel-specific defaults are given in the 'Appendix A' tab of the workbook. The tab 'Appendix B' contains a calculator that can be used to derive custom carbon content factors and Appendix C contains commonly used conversion ratios that should assist users express their data in the expected units.

Caution: Please ensure that the carbon content factor and the fuel requirement emission factor are expressed using either (Lower Heating Value) LHV or (Higher Heating Value) HHV data, and not a mix of both. The LHV is also known as the Net Calorific Value (NCV), while the HHV is also known as the Gross Calorific Value (GCV). Heating values describe the amount of energy released when a fuel is burned completely, and LHVs and HHVs represent different methods to measure the amount energy released. The HHV is the heat evolved when all of the products of combustion are cooled to atmospheric temperature and pressure. The LHV is the heat evolved when the products of combustion are cooled so that water remains as a gas. A given fuel will, therefore, always have two heating value numbers, a LHV and a HHV number. Whereas HHVs are typically used in the US and in Canada, all other countries use LHVs. The LHV of a solid or liquid fuel is approximately 95% that of that fuel's HHV, whereas the LHV of a gaseous fuel, such as natural gas, is about 90% of that fuel's HHV.

5. Enter the amount of CO₂ that is sequestered within CSS technologies and for urea production into Columns G and H respectively.

IV. Quality control

To identify calculation errors and omissions, it is recommended to follow general guidelines provided in Chapter 8 of GHG Protocol for implementing a quality assurance process for all emission estimates. For ammonia production, activity data, emission factors, and calculations can be verified using a variety of approaches:

• Compare the results with emissions data calculated for the same facility in previous years. A calculation error is probable if differences between current data and data from previous years cannot be explained by changes in activity levels, or fuel switching. Also, if the calculation process involved conversion of fuel use data and emission factors, you might want to go back and double check whether no conversion mistakes occurred.

• Data on fuel consumed by specific sources or facilities can be compared with fuel purchasing data.

• If emission estimates were obtained from CEMS, this data can be compared to emissions estimated using the fuel analysis approach.

• If any emission factors were calculated or obtained from the fuel supplier, these factors can be compared to national or international default emission factors.

Uncertainty Assessment

The accuracy of estimating emissions from fossil fuel use in ammonia production is almost entirely determined by the availability of data on the amount of fuel consumed or purchased. If the energy content of the fuels is directly measured or metered, then the resulting uncertainty should be fairly low. Uncertainty increases if it is necessary to convert fuel data measured in mass or volume to energy units. It further increases if dollar amounts of fuels are used to estimate fuel consumption. The primary uncertainty associated with fuel purchasing data is the amount of fuel purchased, but not used. This can result in an overestimate of emissions.

Uncertainty surrounding emission factors is mainly due to the accuracy in which they are measured, and the variability in the supply source.

V. Reporting and Documentation

In order to ensure that estimates are verifiable, the following documentation should be maintained. This information should be collected for auditing and certification purposes, but is not required to be reported or provided.

Data

Documentation source

Fuel consumption data

Purchase receipts, delivery receipts, contract purchase or firm purchase records, stock inventory documentation, metered fuel documentation

Heat contents and emission factors used other than defaults provided

Purchase receipts; delivery receipts; contract purchase or firm purchase records; IPCC, IEA, national or industry reports, test reports

Prices used to convert currency of fuel purchased to amount or energy content of fuel consumed Purchase receipts; delivery receipts; contract purchase or firm purchase records; IPCC, IEA, national or industry reports

All assumptions made in estimating fuel consumption, heat contents, and emission factors All applicable sources

The guidance on external reporting is provided in Chapter 10 of the GHG Protocol.

VI. References

EFMA (2000) Personal Communication with Mr Hans Van Balken, European Fertilizer Manufacturers Association

EPA (1993), *Synthetic Ammonia*, AP-42, 5th ed., Volume 1, Chapter 8, Environmental Protection Agency

IPCC (2006), 2006 IPCC Guidelines for National Greenhouse Gas Inventories Norsk Hydro (2000), Personal communication with Mr Tom Hallan