CHAPTER 3

CHEMICAL INDUSTRY EMISSIONS

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Sections 3.3

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3 CHEMICAL INDUSTRY EMISSIONS

Users are expected to go to Mapping Tables in Annex 5, before reading this chapter. This is required to correctly understand both the refinements made and how the elements in this chapter relate to the corresponding chapter in the 2006 IPCC Guidelines.

3.1 INTRODUCTION

No refinement.

3.2 AMMONIA PRODUCTION

No refinement.

3.3 NITRIC ACID PRODUCTION

3.3.1 Introduction

No refinement.

3.3.2 Methodological issues

Introduction – No refinement.

3.3.2.1 CHOICE OF METHOD

No refinement.

3.3.2.2 CHOICE OF EMISSION FACTORS

TIER 1 METHOD

It is *good practice* to use the highest emission factor based on the technology type shown in Table 3.3 and to assume that there is no abatement of nitrous oxide (N_2O) emissions.

TIER 2 METHOD

If plant-level factors are not available, it is *good practice* to use default factors. These default values often represent midpoint or mean values of data sets (as determined by expert analysis). The extent to which they represent a specific plant's emission rate is unknown. Default factors in Table 3.3 should be used only in cases where plant-specific measurements are not available.

Table 3.3 includes emission factors for N_2O, and associated uncertainties by type of production process.

The five production process types are distinguished according to the pressures applied in the oxidation and absorption stage as presented in Table 3.3a (new).

TABLE 3.3A (NEW)
DIFFERENT PLANT TYPES FOR THE PRODUCTION OF HNO_3[1]

Type	Operation Condition	Applied Pressure in Bar	
		Oxidation	Absorption
L/L	Single Low Pressure	0 - 1.7	
L/M	Dual Low/Medium Pressure	<1.7	1.7 – 6.5
M/M	Single Medium Pressure	1.7 - 6.5	
M/H	Dual Medium/High Pressure	1.7 – 6.5	6.5 - 13
H/H	Single High Pressure	6.5 - 13	

Source:

[1] EC, 2007 (with reference of EFMA, 2000 and Schöffel, 2001)

The factors listed in Table 3.3 for plants using abatement technology, incorporate the effect of N_2O abatement measures. To use these factors, inventory compilers should verify that the abatement technology is installed at individual plants and operated throughout the year.

TABLE 3.3 (UPDATED)
DEFAULT FACTORS FOR NITRIC ACID PRODUCTION

Production Process	N_2O Emission Factor (relating to 100 percent pure acid)
Old (pre-1975) plants* (all processes)	10-19 kg N_2O/tonne nitric acid[a]
Single low pressure plants	5 kg N_2O/tonne nitric acid ±10%
Single medium pressure plants	8 kg N_2O/tonne nitric acid ±20%[b]
Single high pressure plants	9 kg N_2O/tonne nitric acid ±40%
Single pressure plants with abatement technology**	2.5 kg N_2O/tonne nitric acid ±10%[b]
Dual Pressure (M/H)	9 kg N_2O/tonne nitric acid ±30%[b]
Dual Pressure (M/H) with abatement technology	2.5 kg N_2O/tonne nitric acid ±20%[b]
Dual Pressure (L/M)	7 kg N_2O/tonne nitric acid ±20%[b]
Dual Pressure (L/M) with abatement technology	1.5 kg N_2O/tonne nitric acid ±10%[b]

Notes:

* Old (pre-1975) plants means that the EF is to be used for the technology that was installed before 1975 and that are still operating.

** Applies to all single pressure plants using all levels of N_2O abatement measures (primary, secondary, tertiary and quaternary). These abatement measures include all levels of abatement such as process-integrated abatement technologies, tailgas N_2O destruction and non-selective catalytic reduction (NSCR, a NOx abatement technology that can also be managed to abate N_2O).

Source:

[a] Based on IPCC, 2000; EC, 2007; and the tests from Clean Development Mechanism (CDM) projects presented in US EPA, 2010.

[b] Based on information from EC, 2007; EC, 2009; 2017 Annex I Party GHG Inventory Submissions; Joint Implementation projects and Clean Development Mechanism projects availables at the UNFCCC web-site.

TIER 3 METHOD

Plant measurements provide the most rigorous data for calculating net emissions (i.e., N_2O generation and destruction factors). Monitoring N_2O emissions from nitric acid production is practical because these are point sources and there are a finite number of production plants. Given currently available technology, instrumentation for sampling and monitoring emission rates do not limit precision or accuracy of the overall measurement. Usually sampling frequency and timing is sufficient to avoid systematic errors and to achieve the desired level of accuracy.

As a general rule, it is *good practice* to conduct sampling and analysis whenever a plant makes any significant process changes that would affect the generation rate of N_2O, and sufficiently often otherwise to ensure that operating conditions are constant. In addition, plant operators should be consulted annually to determine the specific destruction technologies employed and confirm their use, since technologies may change over time. Precise measurement of the emissions rate and abatement efficiencies requires measurement of both the exit stream and the uncontrolled stream. Where measurement data are available only on the exit stream, *good practice* is to base emissions on these data. In this case, any available estimates of abatement efficiency should be provided only for information purposes and are not used to calculate emissions.

3.3.2.3 CHOICE OF ACTIVITY DATA

No refinement.

3.3.2.4 COMPLETENESS

No refinement.

3.3.2.5 DEVELOPING A CONSISTENT TIME SERIES

No refinement.

3.3.3 Uncertainty assessment

No refinement.

3.3.4 Quality Assurance/Quality Control (QA/QC), Reporting and Documentation

No refinement.

3.4 ADIPIC ACID PRODUCTION

No refinement.

3.5 CAPROLACTAM, GLYOXAL AND GLYOXYLIC ACID PRODUCTION

No refinement.

3.6 CARBIDE PRODUCTION

No refinement.

3.7 TITANIUM DIOXIDE PRODUCTION

No refinement.

3.8 SODA ASH PRODUCTION

No refinement.

3.9 PETROCHEMICAL AND CARBON BLACK PRODUCTION

No refinement.

3.10 FLUOROCHEMICAL PRODUCTION

3.10.1 HFC-23 emission from HCFC-22 production

3.10.1.1 INTRODUCTION

No refinement.

3.10.1.2 METHODOLOGICAL ISSUES

CHOICE OF METHOD

There are two broad measurement approaches to estimating HFC-23 emissions from HCFC-22 plants. These are described in IPCC (2000), DEFRA (2002a and 2002b), EFCTC (2003) and UN (2004) and have been translated into Tier 2 and 3 methodologies described below. National emissions using either of these methodologies are the sum of those from the individual facilities. Tier 1 (default) methodology can be applied to individual plants or, if there is no abatement by destruction, to the total national output of HCFC-22. Accounting for HFC-23 emissions is not simply mechanistic but requires information on the process operations responsible for producing and emitting HFC-23, so that the most appropriate methodology and factors can be adopted. Therefore, it is *good practice*, to the extent possible, to establish contacts with plant managers in order to obtain the necessary data.

The Tier 1 method is relatively simple, involving the application of a default emission factor to the quantity of HCFC-22 produced. This method can be applied at the plant level or the national level. Tier 2 and Tier 3 methodologies are suitable only for plant level calculations because they rely on data that are only available from plants. In cases where there are Tier 3 data available for some plants, the Tier 1 or Tier 2 methods can be applied to the remainder to ensure complete coverage.

It is *good practice* to estimate national emissions by summing measured parameters from all HCFC-22 plants in a country. Tier 3 plant emission measurements are the most accurate, followed by Tier 2 measurements based on plant efficiencies. Direct measurement is significantly more accurate than Tier 1 because it reflects the conditions specific to each manufacturing facility. In most cases, the data necessary to prepare Tier 3 estimates should be available because facilities operating to good business practice perform regular or periodic sampling of the final process vent or within the process itself as part of routine operations. The Tier 1 (default) method should be used only in cases where plant-specific data are unavailable and this subcategory is not identified as significant subcategory under *key category*. (See Section 4.2 of Volume 1.) Modern plant using process optimization will need to keep accurate HFC-23 generation data as part of this optimization, so plant-specific data should be available to most countries in most cases.

The choice of *good practice* method will depend on national circumstances. The decision tree in Figure 3.16 describes *good practice* in adapting the methods in these Guidelines to country-specific circumstances.

Procedures to abate emissions include destruction of HFC-23 in a discrete facility and, in this case, emissions occur only when the destruction facility is not in operation. The tiers of methodology provide estimates for the quantity of HFC-23 that is produced and the share of production that is ultimately emitted depends on the length of time that the destruction facility is not operated. For facilities using abatement techniques such as HFC-23 destruction, verification of the abatement efficiency is also done routinely. It is *good practice* to subtract abated HFC-23 emissions from national estimates where the abatement has been verified by process records on every plant.

Tier 1

In the Tier 1 methodology, a default factor is used to estimate production (and potential emissions) of HFC-23 from the total HCFC-22 production from each facility (for both potentially dispersive uses, as reported under the Montreal Protocol, and feedstock uses, which are reported separately to the Ozone Secretariat). See Equation 3.30.

EQUATION 3.30
TIER 1 CALCULATION OF HFC-23 FROM HCFC-22 (PRODUCED) USING DEFAULT FACTOR

$$E_{HFC-23} = EF_{default} \bullet P_{HCFC-22}$$

Where:

E_{HFC-23} = by-product HFC-23 emissions from HCFC-22 production, kg

$EF_{default}$ = HFC-23 default emission factor, kg HFC-23/kg HCFC-22

$P_{HCFC-22}$ = total HCFC-22 production, kg

This methodology is suitable where plant-specific measurements are not available and, in that case, the default condition is that all of the estimated HFC-23 production is released into the atmosphere.

Tier 2

In the Tier 2 methodology, the HFC-23 emission factor is derived from records of process efficiencies and used in the calculation shown as Equation 3.31. This is a material balance approach and relies on calculating the difference between the expected production of HCFC-22 and the actual production and then assigning that difference to loss of raw materials, loss of product (HCFC-22) and conversion to by-products, including HFC-23. These parameters will be different for each plant and so should be assessed separately for each facility reporting into the national data.

EQUATION 3.31
TIER 2 CALCULATION OF HFC-23 FROM HCFC-22 (PRODUCED) USING FACTOR(S) CALCULATED FROM PROCESS EFFICIENCIES

$$E_{HFC-23} = EF_{calculated} \bullet P_{HCFC-22} \bullet F_{released}$$

Where:

E_{HFC-23} = by-product HFC-23 emissions from HCFC-22 production, kg

$EF_{calculated}$ = HFC-23 calculated emission factor, kg HFC-23/kg HCFC-22

$P_{HCFC-22}$ = total HCFC-22 production, kg

$F_{released}$ = Fraction of the year that this stream was released to atmosphere untreated, fraction

The emission factor can be calculated from both the carbon efficiency (Equation 3.32) and the fluorine efficiency (Equation 3.33) and the value used in Equation 3.31 should normally be the average of these two values unless there are overriding considerations (such as a much lower uncertainty of one of the efficiency measures) that can be adequately documented. Annual average carbon and fluorine balance efficiencies are features of a well-managed HCFC-22 plant and are either normally available to the plant operator or may be obtained by examination of process accounting records. Similarly, if there is a vent treatment system, the length of time that this was in operation, and treating the vent stream from the HCFC-22 plant, should be available from records.

Total HCFC-22 production includes material that is used as a chemical feedstock as well as that which is sold for potentially dispersive uses.

EQUATION 3.32
CALCULATION OF HFC-23 EMISSION FACTOR FROM CARBON BALANCE EFFICIENCY

$$EF_{carbon\_balance} = \frac{(100 - CBE)}{100} \bullet F_{efficiency\ loss} \bullet FCC$$

Where:

$EF_{carbon\_balance}$ = HFC-23 emission factor calculated from carbon balance efficiency, kg HFC-23/kg HCFC-22

CBE = carbon balance efficiency, percent

$F_{efficiency\ loss}$ = factor to assign efficiency loss to HFC-23, fraction

FCC = factor for the carbon content of this component (= 0.81), kg HFC-23/kg HCFC-22

and

EQUATION 3.33
CALCULATION OF HFC-23 EMISSION FACTOR FROM FLUORINE BALANCE EFFICIENCY

$$EF_{fluorine\_balance} = \frac{(100 - FBE)}{100} \bullet F_{efficiency\ loss} \bullet FFC$$

Where:

$EF_{fluorine\_balance}$ = HFC-23 emission factor calculated from fluorine balance efficiency, kg HFC-23/kg HCFC-22

FBE = fluorine balance efficiency, percent

$F_{efficiency\ loss}$ = factor to assign efficiency loss to HFC-23, fraction

FFC = factor for the fluorine content of this component (= 0.54), kg HFC-23/kg HCFC-22

The factor to assign the efficiency loss to HFC-23 is specific to each plant and, if this method of calculation is used, the factor should have been established by the process operator. By default, the value is 1; that is all of the loss in efficiency is due to co-production of HFC-23. In practice, this is commonly the most significant efficiency loss, being much larger than losses of raw materials or products.

The factors for carbon and fluorine contents are calculated from the molecular compositions of HFC-23 and HCFC-22 and are common to all HCFC-22 plants at 0.81 for carbon and 0.54 for fluorine.

Tier 3

Tier 3 methodologies are potentially the most accurate. The Tier 3 methodologies provided here give equivalent results and the choice between them will be dictated by the information available in individual facilities. In each case, the national emission is the sum of factory specific emissions, each of which may be determined using a Tier 3 method to estimate the composition and flowrate of gas streams vented to atmosphere (either directly and continuously – as in Tier 3a - or by continuous monitoring of a process parameter related to the emission - Tier 3b - or by monitoring the HFC-23 concentration continuously within the reactor product stream - Tier 3c):

EQUATION 3.34
TIER 3A CALCULATION OF HFC-23 EMISSIONS FROM INDIVIDUAL PROCESS STREAMS (DIRECT METHOD)

$$E_{HFC-23} = \sum_i \sum_j \int_t C_{ij} \bullet f_{ij} \quad [\textstyle\int_t \text{ means the quantity should be summed over time.}]$$

Where:

E_{HFC-23} = total HFC-23 emissions: the sum over all *i* plants, over all *j* streams in each plant of the emitted mass flows *f* and concentrations *C* is integrated over time *t*. (See Equation 3.37 for calculation of 'instantaneous' HFC-23 emissions in an individual process stream.)

or, where an emission factor-based methodology is used:

EQUATION 3.35 (UPDATED)
TIER 3B CALCULATION OF HFC-23 EMISSIONS FROM INDIVIDUAL PROCESS STREAMS USING A SITE- OR PROCESS-SPECIFIC EMISSION FACTOR

$$E_{HFC-23} = \sum_i \int_t C_i \bullet P_i \quad [\textstyle\int_t \text{ means the quantity should be summed over time.}]$$

Where:

E_{HFC-23} = total HFC-23 emissions: $E_{i,j}$ are the emissions from each plant and stream determined using an emission factor. (See Equation 3.38 for calculation of HFC-23 emissions in an individual process stream.)

or, where the HFC-23 concentration within the reactor product stream is used:

EQUATION 3.36
TIER 3C CALCULATION OF HFC-23 EMISSIONS FROM INDIVIDUAL PROCESS STREAMS (BY MONITORING REACTOR PRODUCT)

$$E_{HFC-23} = \sum_i \int_t C_i \bullet P_i \qquad [\textstyle\int_t \text{ means the quantity should be summed over time.}]$$

Where:

E_{HFC-23} = total HFC-23 emissions: P_i is the mass flow of HCFC-22 product from the plant reactor at the plant *i*, and C_i is the concentration of HFC-23 relative to the HCFC-22 product at the plant *i*. (See Equation 3.40 for calculation of HFC-23 emissions at an individual facility by in-process measurement.)

Tier 3a

The Tier 3a method is based on frequent or continuous measurement of the concentration and flow-rate from the vent at an individual plant. So that the quantity emitted to atmosphere is the mathematical product of the mass concentration of the component in the stream, the flowrate of the total stream (in units compatible with the mass concentration) and the length of time that this flow occurred:

EQUATION 3.37
TIER 3A CALCULATION OF 'INSTANTANEOUS' HFC-23 EMISSIONS IN AN INDIVIDUAL PROCESS STREAM (DIRECT METHOD)

$$E_{ij} = C_{ij} \bullet f_{ij} \bullet t$$

Where:

E_{ij} = 'instantaneous' HFC-23 emissions from process stream *j* at plant *i*, kg

C_{ij} = the concentration of HFC-23 in the gas stream actually vented from process stream *j* at plant *i*, kg HFC-23/kg gas

f_{ij} = the mass flow of the gas stream from process stream *j* at plant *i* (generally measured volumetrically and converted into mass flow using standard process engineering methods), kg gas/hour

t = the length of time over which these parameters are measured and remain constant, hours

If any HFC-23 is recovered from the vent stream for use as chemical feedstock, and hence destroyed, it should be discounted from this emission; material recovered for uses where it may be emitted may be discounted here, if the emissions are included in the quantity calculated by the methods in Chapter 7. Because emissions are measured directly in this tier, it is not necessary to have a separate term for material recovered, unlike Tiers 3b and 3c.

The total quantity of HFC-23 released is then the annual sum of these measured instantaneous releases. Periods when the vent stream is processed in a destruction unit to remove HFC-23 should not be counted in this calculation. If it is necessary to estimate the quantity destroyed at each facility, the operator should calculate this based on the difference between the operating time of the plant and the duration of release (*t* above).

Tier 3b

In many cases, measurements are not continuous but were gained during an intensive process survey or plant trial, and the results of the trial may be used to provide an emission factor for calculating emissions during normal plant operation. In this case, the emission rate of the by-product is related to a more easily (or accurately) measurable parameter, such as feedstock flow rate. The trial(s) must meet the following conditions:

- There should have been no major process design, construction or operating changes that affect the plant upstream of the measurement point and so could render relationships between emissions and production invalid. (See also Box 3.14)
- The relationship between emissions and plant operating rate must be established during the trial(s), together with its uncertainty.

For almost all cases the rate of plant operation is a suitable process operating parameter and the quantity of HFC-23 emitted depends on the current plant operating rate and the length of time that the vent flow was released.

EQUATION 3.38 (UPDATED)
TIER 3B CALCULATION OF HFC-23 EMISSIONS IN AN INDIVIDUAL PROCESS STREAM USING A SITE- OR PROCESS-SPECIFIC EMISSION FACTOR

$$E_{ij} = S_{ij} \bullet F_{ij} \bullet POR_{ij} \bullet t - R_{ij}$$

Where:

E_{ij} = the mass emission of HFC-23 in vent stream *j* at plant *i*, kg

S_{ij} = the standard mass emission factor of HFC-23 in vent stream *j* at plant *i* per 'unit' of a process operating parameter, such as process operating rate (described in Equation 3.39, below), kg/'unit'

F_{ij} = a dimensionless factor relating the measured standard mass emission rate to the emission rate at the actual plant operating rate. In many cases, the fraction produced is not sensitive to operating rate and F_i is unity (i.e., the emission rate is proportional to operating rate). In other cases the emission rate is a more complex function of the operating rate. In all cases F_i should be derived during the plant trial by measuring HFC-23 production at different operating rates. For situations where a simple function relating the emissions to the operating rate cannot be determined from testing, the emission factor-based method is not considered appropriate and continuous measurement is desirable.

POR_{ij} = the current process operating rate applicable to vent stream *j* at plant *i* averaged over *t* in 'unit/hour'. The units of this parameter must be consistent between the plant trial establishing the standard emission rate and the estimate of ongoing, operational emissions (described in Equation 3.39, below).

t = the actual total duration *of venting* for the year, or the period if the process is not operated continuously in hours. Annual emissions become the sum of all the periods during the year. The periods during which the vent stream is processed in a destruction system should not be counted here.

R_{ij} = the quantity of HFC-23 recovered for vent stream *j* at plant *i* for use as chemical feedstock, and hence destroyed, kg. Material recovered for uses where it may be emitted potentially may be counted here if the emissions are included in the quantity calculated by the methods for ODS substitutes in Chapter 7 of this volume.

EQUATION 3.39 (UPDATED)
TIER 3B CALCULATION OF STANDARD EMISSION FOR EMISSION FACTOR-BASED METHOD

$$S_{T,ij} = C_{T,ij} \bullet f_{T,ij} \,/\, POR_{T,ij}$$

Where (for each test T):

S_{ij} = the standard mass emission factor of HFC-23 in vent stream j at plant i, kg/'unit' (in units compatible with the factors in Equation 3.38, see $POR_{T,ij}$ below)

$C_{T,ij}$ = the average mass fractional concentration of HFC-23 in vent stream j at plant i during the trial, kg/kg

$f_{T,ij}$ = the average mass flowrate of vent stream j at plant i during the trial, kg/hour

$POR_{T,ij}$ = the process operating parameter (such as process operating rate) at plant i during the trial, 'unit'/hour. The 'unit' depends on the process operating parameter chosen to be representative for plant i vent stream j (for example, kg/hour or m^3/hour of feedstock)

Tier 3c

It is a relatively simple procedure to monitor the concentration of HFC-23 in the product of a reaction system relative to the amount of HCFC-22. This provides a basis for estimation of the quantity of HFC-23 released as the mathematical product of the monitored concentration and the mass flow of HCFC-22 made. If there is no vent treatment to abate emissions, this is a simple procedure. However, where there is abatement then it must be shown that this actually treats all streams that may be released into the atmosphere, including direct gas vents and the outgassing of aqueous streams. The latter, especially, may not be passed to the destruction facility. If all potential vent streams are not treated, the method cannot be used.

EQUATION 3.40
TIER 3C CALCULATION OF HFC-23 EMISSIONS FROM AN INDIVIDUAL FACILITY BY IN-PROCESS MEASUREMENT

$$E_i = C_i \bullet P_j \bullet t_F - R_i$$

Where:

E_i = HFC-23 emissions from an individual facility i, kg

C_i = the concentration of HFC-23 in the reactor product at facility i, kg HFC-23/kg HCFC-22

P_i = the mass of HCFC-22 produced at facility i while this concentration applied, kg

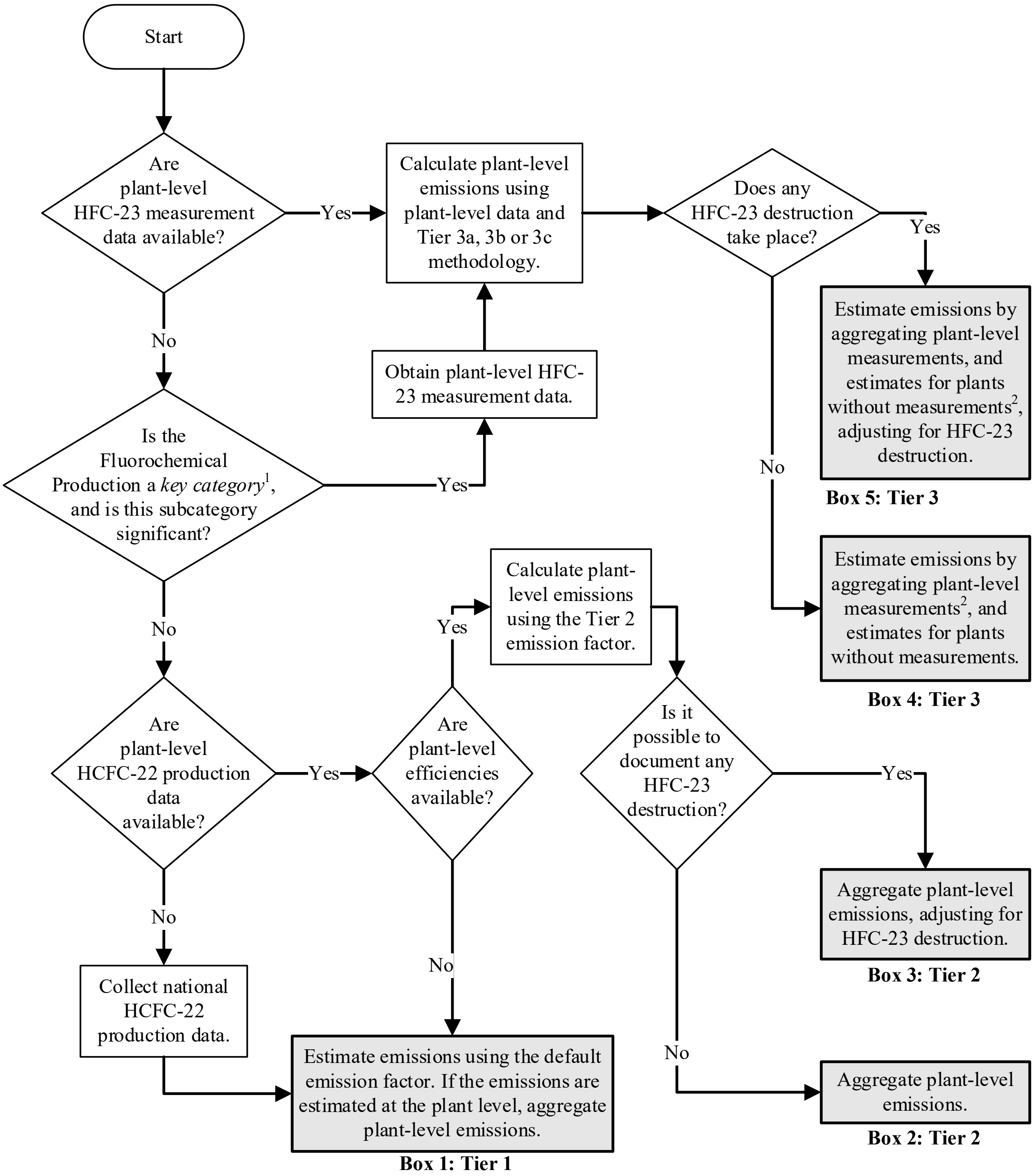
t_F = the fractional duration during which this HFC-23 is actually vented to the atmosphere, rather than destroyed, fraction

R_i = the quantity of HFC-23 recovered from facility i for use as chemical feedstock, and hence destroyed, kg. Material recovered for uses where it may be emitted potentially may be counted here if the emissions are included in the quantity calculated by the methods in Chapter 7 of this volume.

The total quantity of HFC-23 released into the atmosphere is the sum of the quantities from the individual release periods and individual reaction systems. HFC-23 that is recovered for use as chemical feedstock should be subtracted from the total quantity estimated here.

In summary, the Tier 1 method is relatively simple, involving the application of a default emission factor to the quantity of HCFC-22 produced. This method can be applied at the plant level or the national level. Tier 2 and Tier 3 methodologies are suitable only for plant level calculations. In cases where there are Tier 3 data available for some plants, the Tier 1 or Tier 2 methods can be applied to the remainder to ensure complete coverage. Uncertainty in the national emission is then calculated using production weighted uncertainties of the individual sources and standard statistical techniques. Regardless of the method, emissions abated should be subtracted from the gross estimate from each plant to determine net emissions before these are added together in the national estimate.

Figure 3.16 Decision tree for HFC-23 emissions from HCFC-22 production (or other similar by-product emissions from fluorochemical production)



Note:
1. See Volume 1 Chapter 4, Methodological Choice and Identification of Key Categories (noting Section 4.1.2 on limited resources), for discussion of *key categories* and use of decision trees.
2. If there are Tier 3 data available for some plants, the Tier 1 or Tier 2 methods can be applied to the remainder to ensure complete coverage.

It is *good practice* to use the Tier 3 method if possible. Direct measurement is significantly more accurate than Tier 1 because it reflects the conditions specific to each manufacturing facility. In most cases, the data necessary to prepare Tier 3 estimates should be available because facilities operating to good business practice perform regular or periodic sampling of the final process vent or within the process itself as part of routine operations. For facilities using abatement techniques such as HFC-23 destruction, verification of the abatement efficiency is also done routinely. The Tier 1 (default) method should be used only in rare cases where plant-specific data are unavailable and this subcategory is not identified as significant subcategory under *key category*. (See Section 4.2 of Volume 1.)

CHOICE OF EMISSION FACTORS

There are several measurement options within the Tier 3 method relating to the location and frequency of the sampling. In general, direct measurement of the emissions of HFC-23 may provide the highest accuracy but continuous or frequent measurement of parameters within the production process area itself may be more pragmatic and can be equally accurate. In both cases, the frequency of measurement must be high enough to represent the variability in the process (e.g., across the life of the catalyst). Issues related to measurement frequency are summarised in Box 3.14, Plant Measurement Frequency. General advice on sampling and representativeness is provided in Volume 1, Chapter 2.

In cases where plant-specific measurements or sampling are not available and Tier 1 methods are used, the default emission factor should be used, assuming no abatement methods. For plants in operation prior to 1995 the default emission factor is 0.04 kg HFC-23/kg HCFC-22 (4 percent) (IPCC, 1996; US EPA, 2001; McCulloch, 2007). This is a default to be used when there are no measurements and describes the output of HFC-23 from a typical HCFC-22 plant in the absence of recovery or destruction of HFC-23. The value is consistent with atmospheric observations of HFC-23 concentrations in the 1978-1995 time period (Oram *et al.,*1998). These showed globally averaged emissions to be equivalent to 2 percent of the total quantity of HCFC-22 produced at a time when significant HFC-23 was being recovered and converted into Halon 1301 (McCulloch, 1992) and abatement was required practice in several countries where there was significant production.

It is possible, by process optimisation, to reduce the production to between 0.015 and 0.03 kg HFC-23/kg HCFC-22 (1.5 to 3 percent) but it is not possible to completely eliminate HFC-23 formation this way (McCulloch, 2007). Furthermore, the extent of the reduction is highly dependent on the process design and the economic environment (measures to reduce HFC-23 can often reduce the process output). In an optimised process HFC-23 production and emissions will, invariably, have been measured; it is not possible to optimise process operation without such measurements and so default values have no meaning in this context for an individual plant. The state of the technological art has been advanced by optimisation of individual plants and that art should have been built into the design of recent plants, suggesting a default emission factor of 0.03 kg HFC-23/kg HCFC-22 (3 percent). These default values have a large uncertainty (in the region of 50 percent). For more accurate assessments, the actual emissions should be determined by Tier 2 or Tier 3 methodology and, if necessary, assigned to previous years using the guidance provided in Chapter 7 of this volume. Should the vent gas be collected for treatment, thermal oxidation has been shown to reduce HFC-23 emission by 99.996 percent (Irving, 2000).

TABLE 3.28 (UPDATED)
HFC-23 DEFAULT EMISSION FACTORS

Technology	Emission Factor (kg HFC-23/kg HCFC-22 produced)
Old, unoptimised plants (e.g., 1940s to 1990/1995)	0.04
Plants of recent design, not specifically optimised	0.03
Global average emissions (1978 - 1995)[1]	0.02
For comparison:	
Optimised large plant- requiring measurement of HFC-23 (Tier 3)	*Down to 0.015*
Plant with effective capture and destruction of HFC-23 (Tier 3)	*Down to zero*

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[1] The global average is calculated from the change in atmospheric concentration of HFC-23. It does not discriminate between plant emissions, which range from nothing to greater than 4 percent of the HCFC-22 production.

BOX 3.14
PLANT MEASUREMENT FREQUENCY

The accuracy and precision of the estimates of annual HFC-23 emissions depend on the number of samples (the frequency of sample collection) together with the accuracy of measurement of flowrates and the extent to which discrete flow measurements can represent the total quantity vented. Since production processes are not completely static, the greater the process variability, the more frequently plants need to measure. As a general rule, sampling and analysis should be repeated whenever a plant makes any significant process changes. Before choosing a sampling frequency, the plant should set a goal for accuracy and use statistical tools to determine the sample size necessary to achieve the goal. For example, a study of HCFC-22 producers indicates that sampling once per day is sufficient to achieve an extremely accurate annual estimate. This accuracy goal should then be revised, if necessary, to take into account the available resources. (RTI, Cadmus, 1998)

CHOICE OF ACTIVITY DATA

When using the Tier 1 method, production data should be obtained directly from producers. There are several ways producers may determine their production levels, including shipment weights and measuring volume-times-density, using flow meters. These data should account for all HCFC-22 production for the year, whether for sale or for use internally as feedstock, and the plant should describe how the HCFC-22 production rate is determined. In some circumstances, producers may consider plant production data to be confidential. For national-level activity data, submission of HCFC-22 production data is already required under the Montreal Protocol.

COMPLETENESS

It should be possible to obtain complete sampling data because there are only a small number of HCFC-22 plants in each country, and it is standard practice for each plant operator to monitor process efficiencies and hence HFC-23 losses, leading to the adoption of Tier 2 methodology. The destruction efficiencies of thermal oxidisers used to abate HFC-23 are generally high (>99 percent) but it is important to establish the composition of the exit gas in order to ensure that account is taken of emissions of fluorinated greenhouse gases from this point.

DEVELOPING A CONSISTENT TIME SERIES

Emission of HFC-23 from HCFC-22 production should be estimated using the same method for the entire time series and appropriate emission factors. If data for any years in the time series are unavailable for the Tier 3 method, these gaps should be filled according to the guidance provided in Volume 1, Chapter 5.

3.10.1.3 UNCERTAINTY ASSESSMENT

TIER 1

Unlike the other Tiers, where uncertainties are based on measurements and statistics, Tier 1 uncertainties are assessed through expert judgement and an error of approximately 50 percent could be considered for Tier 1 based upon knowledge of the variability in emissions from different manufacturing facilities. An error of this magnitude will completely outweigh the uncertainty in the activity.

TIER 2

Uncertainty of the Tier 2 result is calculated by the root-squared sum of the individual uncertainties in production mass quantity and efficiencies, assuming the carbon and fluorine uncertainties are the same. Where the uncertainties in carbon and fluorine efficiency differ significantly (enough to cause a material difference to the calculated emission), the value with the lower uncertainty should be used throughout the calculation.

Uncertainty in the value derived by Tier 2 methods is much larger than that expected from Tier 3 but is, nevertheless, quantifiable. Typically, for a plant producing about 4 percent HFC-23, the carbon efficiency is in the region of 95 percent and the fluorine efficiency 92 percent. If these efficiencies can be measured to within 1 percent, then the error in the Tier 2 HFC-23 estimate would be less than 20 percent. Estimating efficiencies to this degree of accuracy will require rigorous accounting procedures and that all raw materials and product for sale should be weighed in or out of the facility. Such a regime sets the expected accuracy of the overall activity (for both Tiers 1 and 2); with good accounting and measurement of production by weight, it should be possible to reduce the error in the activity to below 1 percent.

TIER 3

For HFC-23, the Tier 3 method is significantly more accurate than either the Tier 2 measured or Tier 1 default methods. Regular Tier 3 sampling of the vent stream can achieve an accuracy of 1-2 percent at a 95 percent confidence level in HFC-23 emissions and the uncertainty of the Tier 3 (emission-factor-based) result may be similar. In both cases, the uncertainty may be calculated statistically from the uncertainties of the input parameters and, because these methods do not rely on emission factors or activities, the concept of subdividing uncertainty has no validity.

Uncertainty of the estimate is expressed as a coefficient of variance (percent) and, for each of these streams, there will be an uncertainty as a consequence of uncertainties in measured concentration and flowrate and uncertainty in the duration of the flow. The combined uncertainty can be determined analytically and should be calculated using the standard methodology described in Chapter 3 of Volume 1.

3.10.1.4 QUALITY ASSURANCE/QUALITY CONTROL (QA/QC), REPORTING AND DOCUMENTATION

No refinement.

3.10.2 Emissions from production of fluorinated compounds (other than HFC-23 emissions from HCFC-22 production)

3.10.2.1 INTRODUCTION

The emission of HFC-23 from HCFC-22 manufacture was considered in Section 3.10.1. Section 3.10.2 (this section) considers emissions from other fluorochemical production processes. These emissions include emissions of the intentionally manufactured chemical as well as reactant and by-product emissions. For example, in a national inventory for a fluorochemical plant, significant by-product emissions of SF_6, CF_4, C_2F_6, C_3F_8, C_4F_{10}, C_5F_{12} and C_6F_{14} were reported (United Nations Framework Convention on Climate Change (UNFCCC), 2005). Other examples include the release of by-product N_2O and CF_4 from the production of NF_3 (Tasaka, 2004; 2007), CF_4 from the production of CFC-11 and 12, or of SF_6 from the production of uranium hexafluoride in the nuclear fuel cycle.

Typically, fluorochemicals may be released from chemical processes involving a broad range of technologies and processes[2]:

- Telomerization Process used in the production of fluorochemicals fluids and polymers;
- Photooxidation of tetrafluoroethylene to make fluorochemical fluids;
- Direct Fluorination often used in SF_6 production;
- Halogen Exchange Processes to make HFCs 134a and 245fa and low-boiling-point PFCs like C_2F_6 and CF_4;
- NF_3 manufacturing by direct fluorination;
- Production of uranium hexafluoride;
- Production of fluorinated monomers like tetrafluoroethylene and hexafluoropropylene;
- Production of fluorochemical agrochemicals;
- Production of fluorochemical anesthetics;
- Production of perfluorpolyethers;
- Production of hydrofluoroolefins (HFO) such as tetrafluoropropene and its precursors.

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[2] This list is illustrative.

Halogen exchange processes are extensively used for HFC manufacture, while most PFCs and SF_6 require elemental fluorine, generated electrochemically. In 'electrochemical fluorination' processes, the fluorine is not separated but makes the desired product in the electrochemical cell. In other processes it is separated and subsequently used, either as the elemental gas or as a component of a carrier system, such as CoF_3. Each process will have a different spectrum of emissions, in terms of both chemical nature and quantities, and so a common default emission function is subject to considerable uncertainty.

Potential sources of fluorinated GHG emissions at fluorochemical production facilities include the following: process vents, equipment leaks, and evacuating returned containers. Production-related emissions of fluorinated GHGs occur from both process vents and equipment leaks. Process vent emissions occur from manufacturing equipment such as reactors, distillation columns, and packaging equipment. Equipment leak emissions, or fugitive emissions, occur from valves, flanges, pump seals, compressor seals, pressure relief valves, connectors, open-ended lines, and sampling connections. In addition, users of fluorinated GHGs may return empty containers (e.g., cylinders) to the production facility for reuse; prior to reuse, the residual fluorinated GHGs (often termed "heels") may be evacuated from the container and are a potential emission source. In many cases, these "heels" are contaminated and are exhausted to a treatment device for destruction. In other cases, however, they are released into the atmosphere. The Tier 1 default emission factor is intended to cover emissions for process vents, equipment leaks, and container venting.

It is essential that the existence of potentially emissive plants is identified within each country; hence this step is first in the decision tree (Figure 3.17). The common factor for most of these plants is the use of anhydrous hydrogen fluoride, which is the source of fluorine in halogen exchange processes and in processes that use elemental fluorine. The production and importation of anhydrous hydrogen fluoride can therefore be used as a means of tracing significant producers of fluorochemicals. Note that in some cases, the plant consuming the anhydrous hydrogen fluoride may be supplying fluorinated feedstocks to other plants that themselves produce fluorochemicals and emit GHGs. Further enquiries (see Figure 3.17) can elucidate whether or not there are significant fluorochemical greenhouse gas emissions at the plant consuming the anhydrous hydrogen fluoride and whether or not that plant supplies fluorinated feedstocks to other plants.

Feedstocks commonly used in the production of fluoropolymers are HCFC-22, 1,1 difluoroethlyene, tetrafluoroethylene (TFE), and hexafluoropropylene oxide (HFPO). Their production and imports can therefore be used to identify significant producers of fluoropolymers that may not themselves be consumers of hydrogen fluoride.

In this section, emissions associated with use are not addressed specifically, being counted in the emissions related to consumption (see Chapters 4.5, 6, 7 and 8 in this volume).

3.10.2.2 METHODOLOGICAL ISSUES

CHOICE OF METHOD

It is *good practice* to choose the method using the decision tree shown in Figure 3.17. If the Category 2B9 Fluorochemical Production is identified as *key* and this subcategory is judged to be significant, inventory compilers should consider whether or not emissions are dominated by the production of a sub-set of chemicals, and focus more sophisticated data collection efforts on production of these chemicals. We estimate that 80 fluorochemical production facilities operate among 20 countries world-wide (2004 SRI report; U.S. Environmental Protection Agency (EPA) Greenhouse Gas Reporting Program (GHGRP)). A survey of national producers should not be difficult to compile.

Tier 1

In the Tier 1 methodology, a default emission factor, or a similar number derived for the particular country's circumstances, can be used to estimate national production-related emissions of individual HFCs, PFCs, SF_6 and other fluorinated greenhouse gases. The default emission factors in Table 3.28a are expressed in terms of kg emitted/kg produced). When used in a Tier 1 calculation, the applicable default emission factor is multiplied by the total mass of fluorinated chemical produced.

EQUATION 3.41
TIER 1 CALCULATION OF PRODUCTION-RELATED EMISSIONS

$$E_k = EF_{default,k} \bullet P_k$$

Where:

E_k = production-related emissions of fluorinated greenhouse gas k, kg

$EF_{default,\,k}$ = default emission factor, kg emitted /kg produced

P_k = total production of fluorinated chemical k, kg

The fluorinated greenhouse gas k could be the intended gas being manufactured, an un-intended by-product formed during manufacturing, or a reactant feed. Problems of confidentiality arising from reporting specific component data can be circumvented by providing a single number for total national emissions of each HFC, PFC, SF_6 or other fluorinated GHG. This may be facilitated if data are collected by a third party and reported only as this total.

Tier 2

A mass balance based approach that is based on process efficiencies can be more complicated than for HFC-23 emissions from HCFC-22 plants as there can be a range of by-products responsible for process inefficiency (unlike the case for HCFC-22 where one by-product predominates), as well as loss of the intended product and reactants. However, production efficiency data should exist for each process and, in the absence of a more rigorous estimate, the emissions can be estimated based on the difference between the total mass of the reactants and that of the products. These emissions can then be characterized based on information regarding the chemical composition of the emitted mass. The chemical composition may be determined based on measurements, engineering calculations and assessments, process knowledge, etc. Such an estimate may enable a qualitative decision as to whether or not these emissions are a significant subcategory under a *key category*. Should sufficient measurements of the chemical composition of the emissions exist, this methodology could also be used for estimating emissions for reporting.

The mass balance method is summarized in Equation 3.41a below. If the chemical composition of the mass of material emitted from the process is determined through chemical analysis (e.g., a sample taken from the laboratory-, pilot-, or full-scale process) the Tier 2 estimate is further improved.

EQUATION 3.41A (NEW)
TIER 2 CALCULATION OF PRODUCTION-RELATED EMISSIONS USING A MASS BALANCE APPROACH

$$E_k = \sum_i \sum_j \int_t C_{ijk} \bullet M_{ij}$$

Where:

E_k = total production-related emissions (kg) of fluorinated greenhouse gas k: the sum over all i plants, over all j streams in each plant and integrated over time t.

C_{ijk} = the concentration of fluorinated greenhouse gas k present in emissions from stream j, at plant i, kg/kg

M_{ij} = mass emitted from stream j, at plant i, as determined from a mass balance. This mass determined from the difference in the mass of materials (products, by-products, or reactants) entering and leaving the process, kg

The mass balance method accounts for both vented and leaked emissions, but not emissions from the venting of returned cylinders. In the case of cylinder venting, emissions can be estimated based on the mass of material vented from the cylinder and the chemical composition of the mass.

Tier 3

The Tier 3 methodology is potentially the most accurate estimate and is the sum of factory specific emissions of *each* fluorinated greenhouse gas (reactants, intended product, and by-products) determined using standard methods to estimate the composition and flowrate of gas streams actually vented to atmosphere after any abatement technology. Selected examples of standard methods are Fourier transform infrared spectroscopy (FTIR), gas chromatography and mass spectrometry (GC/MS), and calibrated mass flow meters. The particular standard method used for measurement is chosen based on the type of manufacturing process being monitored. As noted above, emissions from manufacturing can be divided into two categories: process vents and equipment leaks. The total emissions of greenhouse gas *k*, from both process vents and equipment leaks is determined as described by Equation 3.41b.~~,~~

EQUATION 3.41B (NEW)
TIER 3 SUMMATION OF PRODUCTION-RELATED EMISSIONS FROM PROCESS VENTS AND EQUIPMENT LEAKS

$$E_k = E_{kPV} + E_{kEL}$$

Where:

E_k = total production-related emissions of fluorinated greenhouse gas k from process vents and equipment leaks

E_{kPV} = total production-related emissions of fluorinated greenhouse gas k from process vents

E_{kEL} = total production-related emissions of fluorinated greenhouse gas k from equipment leaks

Process vent and equipment leaks are described as follows.

Process Vents

Process vents are typically configured for intermittent or continuous measurement(s) of the concentration, and where a process-vent flow rate exists, emissions can be determined as follows:

EQUATION 3.42 (UPDATED)
TIER 3 DIRECT CALCULATION OF PRODUCTION-RELATED EMISSIONS FROM PROCESS VENTS

$$E_{kPV} = \sum_i \sum_j \int_t C_{ijk} \bullet f_{ijk}$$

Where:

E_{kPV} = total process vent, production-related emissions of fluorinated greenhouse gas k: the sum over all i plants, over all j streams in each plant of the emitted mass flows f and concentrations C and integrated over time t.

Alternatively, process vent emissions can be determined by utilizing a facility- or process-specific emission factor. The emission factor is determined by normalizing the emission rate of the reactants, intended product, and by-products by a more easily (or accurately) measurable parameter, such as feedstock flow rate, as described in Equation 3.38 in Section 3.10.1:

EQUATION 3.43 (UPDATED)
TIER 3 CALCULATION OF PRODUCTION-RELATED EMISSIONS FROM PROCESS VENTS USING A SITE- OR PROCESS-SPECIFIC EMISSION FACTOR

$$E_{kPV} = \sum_i \sum_j \int_t E_{ijk}$$

Where:

E_{kPV} = total process vent, production-related emissions of fluorinated greenhouse gas k: summed over all i plants, over all j streams and integrated over time t.

E_{ijk} = the process vent emissions of fluorinated greenhouse gas k from each plant and stream determined by the facility- or process- specific emission factor based methods, described in Equations 3.38 and 3.39 in Section 3.10.1

For process vents, emissions may be determined based on direct measurements, engineering calculations and assessments, and process knowledge. For continuous processes with significant fluorinated GHG emissions, it is *good practice* to develop site-specific or even process-vent-specific emission factors based on measurements of emissions and activity. For smaller processes and for batch processes, it is *good practice* to develop the specific emission factors based on either measurements or engineering calculations and assessments. Note that, generally, flows are measured volumetrically and should be converted into mass flow (kg/hour) based on the ideal gas law, temperature, pressure and composition; similarly concentration should be converted into compatible units (e.g., kg/kg).

In this case, the flowrates, concentrations and duration should be calculated separately for the periods when the abatement technology is or is not operating and only those that lead to actual emissions should be summed and reported.

Cylinder Venting

In the case of cylinder venting, the Tier 3 approach uses the mass of material vented from the cylinder and the chemical composition of the mass as the basis for the emissions estimate. The chemical composition is typically available from the contents of the cylinder (e.g., stated purity or certificate of analysis). If there is a question regarding the composition of the cylinder contents (e.g., anticipate that impurities are present), then the Tier 3 approach may include actual measurement of the chemical composition of the vented material using an analytical method specified previously in this section.

Equipment Leaks

Emissions from equipment leaks can originate from a variety of process and equipment types; there are a number of different standard methods from which to choose. Three example approaches follow and are based on guidance from US EPA (1995): the Screening Ranges Approach, Correlation Approach, and Unit-Specific Correlation Approach. While these approaches were developed for hydrocarbons primarily, similar equipment is used for fluorochemical production, transfer, and storage and they are therefore appropriate for fluorochemicals. The choice of equipment component used is mostly based on the physical state of the chemical (gas, liquid) and the temperature and pressure of the process stream. For a given set of physical parameters, differences in the chemical properties between hydrocarbon and fluorochemicals are not expected to significantly affect the leak rate from valves, flanges, seals, etc. (See section 2.4.1, 2.4.6, and 2.4.7 in EPA, 1995 for additional information on speciating emissions.) It is, however, important to use appropriate monitoring equipment capable of measuring fluorinated chemicals. For all three approaches, fluorochemicals typically have dramatically different response factors than hydrocarbons, and in some cases, have little response on analytical equipment commonly used for hydrocarbon leak detection.

In the Screening Ranges Approach, two sets of emission factors are combined with corresponding equipment counts to estimate emissions. Emission factors are assigned to pieces of equipment (sources) based on whether a leak detector applied to the source indicates fluorinated GHG concentrations fall above (source greater than, or SG) or below (source less than, or SL) a particular leak concentration definition. These definitions are available from US EPA (1995) for many types of equipment (these US EPA values are for total organic compounds but may be applied to fluorinated GHG).

EQUATION 3.43A (NEW)
TIER 3 CALCULATION OF EMISSIONS FROM EQUIPMENT LEAKS USING A SCREENING RANGES APPROACH

$$E_{gijkEL} = (SG_{ig} \bullet CG_{ig} \bullet C_{gijk}) + (SL_{ig} \bullet CL_{ig} \bullet C_{gijk})$$

Where:

E_{gijkEL} = the equipment leak–related emissions of fluorinated greenhouse gas k in stream j, from plant i, from equipment type g, kg/hr.

SG_{ig} = applicable emission factor for sources with screening values greater than or equal to 10,000 ppmv from equipment type *g* at plant i, kg/hr-source

CG_{ig} = equipment count for sources with screening values greater than or equal to 10,000 ppmv

from equipment type g at plant i.

C_{gijk} = the concentration of fluorinated greenhouse gas k, present in emissions leaking from equipment type g, in stream j, from plant i, kg/kg or L/L

SL_{ig} = applicable emission factor for sources with screening values less than or equal to 10,000 ppmv from equipment type g at plant i, kg/hr-source.

CL_{ig} = equipment count for sources with screening values less than or equal to 10,000 ppmv from equipment type g at plant i.

Use of the actual screening value measurements where available (i.e., the actual concentration in ppm, not only an indication of above or below 10,000 ppmv), with the Correlation Approach is an additional refinement to the Screening Ranges approach. The Correlation Approach utilizes correlations developed by the US EPA (1995) to predict mass emission rate as a function of screening value for a particular equipment type. Equipment types include gas valves, light liquid valves, connectors, and light liquid pump seals.

EQUATION 3.43B (NEW)
TIER 3 CALCULATION OF EMISSIONS FROM EQUIPMENT LEAKS USING A CORRELATION APPROACH

$$E_{gijkEL} = (Slope_g \bullet (SV_{gjk})^{CE_g}) \bullet C_{gijk})$$

Where:

E_{gijkEL} = the equipment leak–related emissions of fluorinated greenhouse gas k, of stream j, from equipment type g, at plant i, kg/hr.

$Slope_g$ = slope of correlation equation for equipment type g. See US EPA (1995).

CE_g = exponent for correlation equation for equipment type g.

SV_{gjk} = screening value for greenhouse gas k, in stream j, from equipment type g.

C_{gijk} = the concentration of fluorinated greenhouse gas k present in emissions leaking from equipment type g, in stream j, from plant i, kg/kg

It is important to ensure the units of the correlation and screening values (SV) are consistent with each other. In the case that the SV value is zero, or the value is higher than the upper limit able to be measured by the portable screening device, default EL_j values in units of kg/hr per equipment type exist.

The third approach for estimating equipment leak emissions is the Unit-Specific Correlation Approach. In the Unit-Specific Correlation Approach, selected mass emission rates are determined by an equipment bagging procedure, and the associated screening value (concentration) is concurrently measured. This set of data is used to develop a unit-specific correlation (i.e., regression equation) between the log base 10 value of the leak/mass rate and screening value for a specific equipment type on a given process unit, as described in Equation 3.43c.

EQUATION 3.43C (NEW)
TIER 3 CALCULATION OF A UNIT-SPECIFIC CORRELATION

$$\log_{10} E_{gijk} = (\beta_0 + \beta_1 \bullet SV_{gijk})$$

Where:

E_{gijkEL} = the equipment leak–related emissions of fluorinated greenhouse gas k, in stream j, and equipment type g, at plant i. kg/hr.

β_0 = intercept of regression equation (determined from the measurements and data gathered using the equipment bagging procedure for the particular equipment).

β_1 = slope of regression equation (determined from the measurements and data gathered using the equipment bagging procedure for the particular equipment).

SV_{gijk} = screening value for greenhouse gas k from in stream j, equipment type g, at plant i.

EQUATION 3.43D (NEW)
TIER 3 CALCULATION OF EMISSIONS FROM EQUIPMENT LEAKS USING A UNIT-SPECIFIC CORRELATION APPROACH

$$E_{gijkEL} = (SBCF_{gijk} \bullet 10^{\beta_0} \bullet (SV_{gijk})^{\beta_1} \bullet C_{gijk})$$

Where:

E_{gijkEL} = the equipment leak–related emissions of fluorinated greenhouse gas k, in stream j, from equipment type g, at plant i. kg/hr.

$SBCF_{gijk}$ = Scale bias correction factor (The SBCF is a function of the mean square error of the correlation in log space, as described in US EPA (1995).

C_{gijk} = the concentration of fluorinated greenhouse gas k present in emissions leaking from stream j, from plant i. kg/kg

The total emissions of greenhouse gas *k*, from equipment leaks is determined as described by Equation 3.43e where emissions are summed over all streams *j*, equipment types *g*, at all plants *i*, over a given time period *t*. Should values of E_{gijk} originate from the Unit-Specific Correlation Approach, special care must be used to ensure that these E_{gijk} are used only for the particular equipment type and plant where they were generated.

EQUATION 3.43E (NEW)
TIER 3 CALCULATION OF PRODUCTION-RELATED EMISSIONS FROM EQUIPMENT LEAKS

$$E_{kEL}=\sum_{i}\sum_{j}\sum_{k}\int_{t}E_{gijkEL}$$

Where:

E_{kEL} = total equipment leak, production-related emissions of fluorinated greenhouse gas k and integrated over time t.

E_{gijkEL} = the equipment leak-related emissions of fluorinated greenhouse gas k in stream j, from plant i, and equipment component type g as determined by the methods, described in Equations 3.43a, 3.43b, or 3.43d.

CHOICE OF EMISSION FACTORS

Tier 1

Tier 1 relies on default emission factors. The default emission factors presented in Table 3.28a are based on a survey of the available literature and, in the case of the last factor, on an analysis of data reported to the US EPA Greenhouse Gas Reporting Program. The first two sets of factors apply to production of SF_6 and NF_3 respectively; the last applies to production of any other fluorochemical. All of the default emission factors assume there is no use of abatement and the default emission factors for SF_6, NF_3, and “other fluorochemicals” include emissions from both process vents and equipment leaks (see Annex 3A.1).

The lower emission factor provided for SF_6 was based on estimated typical emission rates during production; the higher emission factor was found for facilities that also vented residual gas (the “heel”) from containers before refilling them (because their customers, electronics manufacturers, required highly purified SF_6 gas). In countries with SF_6 production, it is *good practice* to apply the lower emission factor if container heels are known to be recycled or destroyed; otherwise, it is *good practice* to apply the higher emission factor.

Both the GHGs emitted and the emission rates for those GHGs (kg per kg of the fluorochemical produced) are shown in the middle column of the table. There is a wide range of substances that may potentially be released during production of fluorochemicals. In some cases, the fluorinated GHGs released during production of a particular fluorochemical have GWPs similar to that of the produced fluorochemical (AFEAS 2004). However, in other cases, the GWPs of the released fluorinated GHGs can be significantly different from that of the produced fluorochemical. The default emission factors presented in Table 3.28a, along with the default composition of emitted fluorinated GHGs in Table 3.28b, reflect both of these situations.

The Tier 1 factors are highly uncertain. Therefore, if emission factors specific to the facility and produced fluorochemical are available, these should be used. Because emission rates vary widely among facilities and processes, caution should be used when applying emission factors measured for a particular fluorochemical at a particular facility to the same fluorochemical at a different facility. However, emission factors measured at other facilities for the same fluorochemical may be used when the process type (see section 3.10.2.1) used to produce the fluorochemical is the same at both facilities, when the treatment of container heels is the same at both facilities, and when the emission factor does not reflect abatement. (Emission factors that reflect abatement should not be used in the Tier 1 method.) Note that an emission factor measured for production of one fluorochemical is not applicable to the production of another, even at the same facility, because different fluorochemicals (even if they are chemically similar, such as two HFCs) are associated with different by-products and different by-product generation rates. Thus, not only the identities, but also the quantities of the GHGs emitted differ.

Some process-specific emission factor data are available from commercially available life cycle assessment software; these emission factors may be used if their source data, calculation methods, and units of measure are well documented.

TABLE 3.28A (NEW)
TIER 1 DEFAULT EMISSION FACTORS FOR FLUOROCHEMICAL PRODUCTION

Fluorochemical Produced	Emission Factor for each Emitted GHG (kg fluorinated GHG emissions/kg fluorochemical produced)	Uncertainty for default emission factor for fluorochemical production
SF_6	0.03 (SF_6)[a] 0.08 (SF_6)[b]	±50% (0.015 to 0.045) ±50% (0.04 to 0.12)
NF_3	0.02 (NF_3)[c] 0.03 (N_2O)[d] 0.01 (CF_4)[d]	±50% (0.01 to 0.03) ±50% (0.015 to 0.045) ±50% (0.005 to 0.015)
All other fluorochemicals	0.04 (see Table 3.28B for composition of emitted mass)[e]	-98% to +470% (0.001 to 0.2)[f]

Source:

[a] O'Connell, 2002.

[b] Suizu, 1999.

[c] Fthenakis, 2010.

[d] Tasaka, 2004; 2007.

[e] As described further in Annex 3A.1 of this Volume, the default emission factor was estimated using data from the US EPA Greenhouse Gas Reporting Program (US EPA, 2017a; 2017b). Briefly, under the Greenhouse Gas Reporting Program, fluorinated GHG emissions are reported annually on a facility basis and include facilities with and without abatement. Depending on the year, 14 to 16 fluorochemical production facilities have reported under the Program. Facilities that abate their emissions report their level of abatement for each process as a range. To develop emission factors on an uncontrolled basis, the pre-abatement emissions of each facility were estimated using the arithmetic averages of the abatement ranges reported by that facility for its processes. Then, for each facility, this estimate was divided by the total quantity of fluorinated gases produced or transformed by that facility to obtain an uncontrolled emission factor for that facility and year. This was done for all six years for which the US EPA had data at the time the factor was developed. For each facility, the emission factors for each year were then averaged over the six years of reporting, and the resulting facility averages were averaged to obtain the default factor above. Because the reporting U.S. facilities use multiple manufacturing methods to produce a wide array of fluorochemicals,[3] averaging the facility-specific emission factors is expected to provide a default emission factor that is applicable where the manufacturing method is unknown, as is often the case in a Tier 1 calculation.

[f] As noted above, emission rates from different manufacturing methods can vary widely, a pattern seen in the variation of the emission factors across the facilities reporting to the U.S. Greenhouse Gas Reporting Program. This variation (summarized here as a 95-percent confidence interval around the arithmetic mean) provides a first order estimate of the uncertainty of the default Tier 1 emission factor. Thus, the default emission factor is broadly applicable, but it is also highly uncertain due to the inherent variability of emission rates across manufacturing methods and produced fluorochemicals.

In addition to the compounds being intentionally produced, a variety of fluorinated GHG by-products can be emitted from fluorochemical manufacturing processes. Emissions of these other fluorinated GHGs can exceed emissions of the compound being intentionally produced. Where the specific fluorinated GHGs emitted are known, inventory compilers should assume that the mass emitted consists of these compounds. Where the specific fluorinated GHGs emitted are not known, it is *good practice* to assume that the mass emitted consists of the fluorinated GHGs listed in Table 3.28b in the proportions provided.

TABLE 3.28B (NEW)
REPRESENTATIVE CHEMICAL COMPOSITION OF THE EMITTED MASS

Fluorinated GHG emitted	Percentage emitted (% of unweighted tonne)[a]
HFC-134a	18
PFC-14 (Perfluoromethane)	18
Perfluorocyclobutane	13
HFC-32	11
HFC-125	11
HFC-23	11

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[3] Fluorochemicals produced in the U.S. and reported to the GHGRP include HFCs, HFEs, PFCs, SF_6, NF_3, other fully fluorinated greenhouse gases, and others. Emissions are also reported from the transformation of some of these substances, as well as CFCs and HCFCs, into other materials such as polymers.

TABLE 3.28B (NEW) (CONTINUED)
REPRESENTATIVE CHEMICAL COMPOSITION OF THE EMITTED MASS

Fluorinated GHG emitted	Percentage emitted (% of unweighted tonne)[a]
HFC-143a	7
PFC-116 (Perfluoroethane)	5
PFC-218 (Perfluoropropane)	4
PFC-5-1-14 (Perfluorohexane, FC 72)	3

Due to rounding, the sum of individual items will not equal 100%.

Source:

[a] To derive this composition, six years of US EPA GHGRP data were sorted, and the chemical species with the highest estimated uncontrolled emissions (in metric tonne) were identified. The weighted average GWP of these emissions is the same as the weighted average GWP of the uncontrolled emissions (other than very low-GWP emissions) estimated for fluorinated gas producers that report to the US EPA.[4] More discussion on the development of the default emissions factor and the representative chemical composition is provided in Annex 3A.1.

Tier 2 and Tier 3

Tier 2 relies on an estimate of the mass of emissions lost from the process, and if available, measurement(s) of the chemical composition of the emitted mass. Tier 3 relies on direct measurements of, and the use of, process- and facility-specific emission factors to determine the quantities of individual fluorinated GHGs released into the atmosphere.

For Tier 2 and Tier 3, it is important to determine and document whether the production facility abates production-related emissions of each fluorinated GHG. If the quantity of gas emitted to the atmosphere is reduced by, for example, thermal treatment of the vent stream, the quantity emitted should be adjusted to account for the destruction efficiency of the oxidiser and the length of time that it is in service. As an example, when a thermal treatment unit is well-operated and well-maintained, it has been shown to reduce HFC-23 emission by 99.996 percent (Irving, 2000). However, the on-line time of the destruction process can also have a significant effect on emissions and should be recorded. For example, in the case of a treatment system with 99 percent removal efficiency, the magnitude of fluorinated GHG emissions would be dominated by the amount of time the gas stream is being treated.

Emission control technologies are used at many facilities to control fluorinated GHG emissions from process vents. Destruction and removal efficiencies (DREs) are generally based on performance testing of emission control devices. Results are expected to vary across process equipment and gas flow rates. To apply a DRE to an emission control device, the device must be specifically designed to abate fluorochemicals. If facilities use other types of abatement devices not designed specifically for fluorinated GHGs, they should assume that its destruction efficiency is 0 percent for fluorinated GHGs. In addition, the inventory compiler must demonstrate through communication with facility managers and subsequent documentation that emissions control technologies are operated and maintained in accordance with manufacturer specifications. The DRE should only apply to that portion of emissions that pass through a properly operating and maintained control device, and DRE should not be applied when control device is bypassed, not operating according to manufacturer specifications, or not maintained in accordance with specifications.

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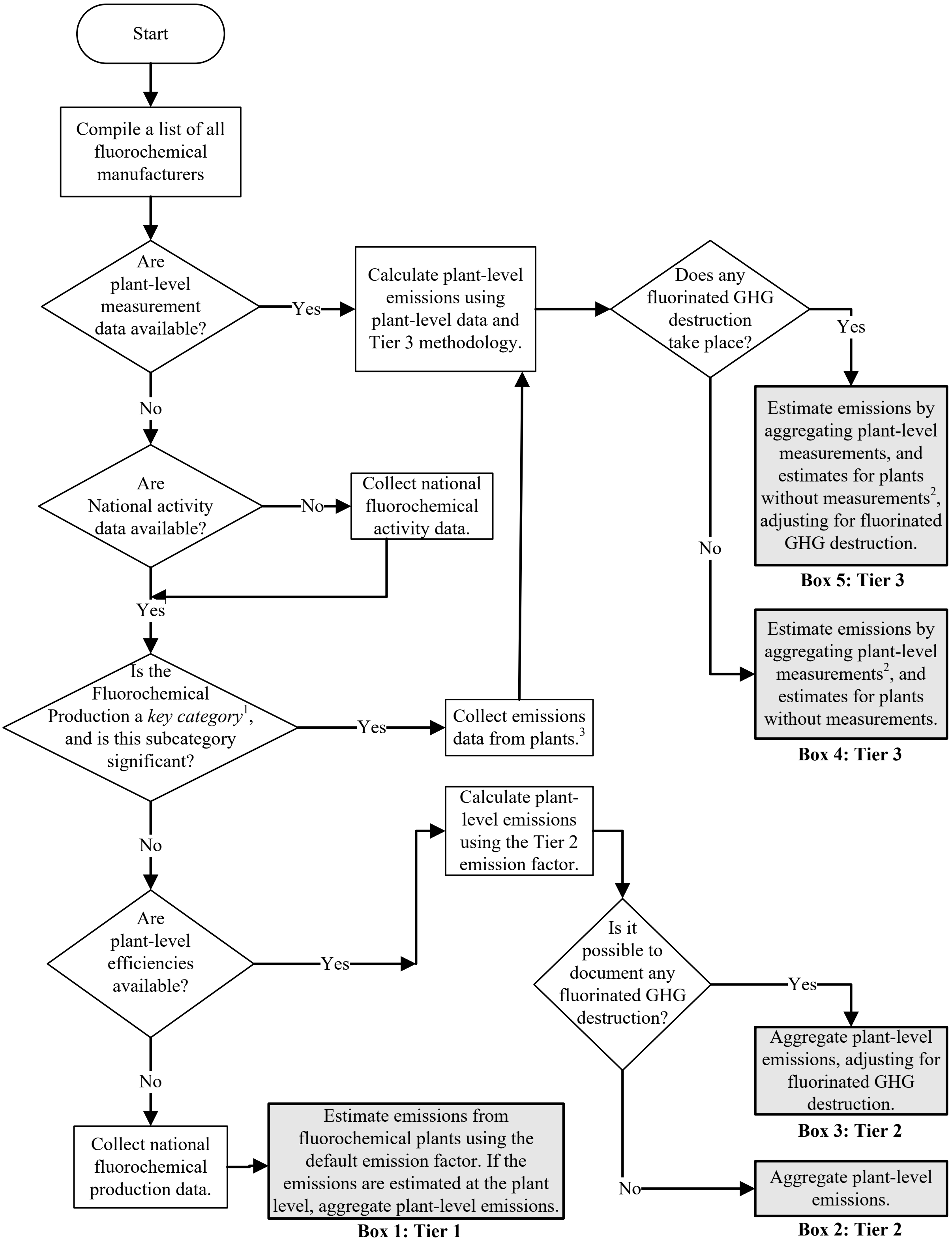
[4] To develop both the mass emission factor in Table 3.28a and the break-out of fluorinated GHGs in Table 3.28b, fluorinated GHGs with GWPs above one were included in the analysis. Fluorinated GHGs with GWPs near one, such as unsaturated HFCs and PFCs, were excluded. This reduced the emission factor in terms of tons emitted/tons produced, but it had negligible impact on the metric tonne of CO_2eq. emitted/metric tonne produced.

Figure 3.17 (Updated) Decision Tree for emissions of fluorinated greenhouse gas from fluorochemical production processes, applicable to product, by-product, reactant, and fugitive



Note:

1. See Volume 1 Chapter 4, Methodological Choice and Identification of *Key Categories* (noting 4.1.2 on limited resources), for discussion of *key categories* and use of decision trees.

2. If there are Tier 3 data available for some plants, the Tier 1 or Tier 2 methods can be applied to the remainder to ensure complete coverage.

3. Data may be collected as a country study by a third party in order to preserve confidentiality.

CHOICE OF ACTIVITY DATA

For Tier 1, the activity is the annual mass of the desired fluorochemical that is produced. These activity data may be available as total production data for the country or may be available for individual facilities. For Tier 2, the activity is the mass of the produced fluorochemical(s) as well as the consumption of feedstocks. For Tier 3, the activity data for emissions from process vents may be either the annual mass of the produced fluorochemical(s) or the annual mass or quantities of one or more feedstocks consumed, and the activity data for emissions from equipment leaks is the number of potentially leaking equipment components of each type. Individual facilities should have access to the activity data for Tier 2 and Tier 3. For Tier 3, the activity data may sometimes be available from an industry trade group.

Recycling

Recycling of used gas may be done by the producers of new gas or by other recycling firms. Emissions may occur during handling and purification of old gas and handling of recycled gas. Specific emission factors are not available. Thus, *good practice* is to use the same default factor as for new production.

COMPLETENESS

Completeness requires that the national GHG inventory include all GHG emissions from all fluorochemical production processes (including emissions from both process vents and equipment leaks) and any other emission sources (including container venting) at all facilities in the country. It is important to note that significant GHG emissions occur not only from processes and facilities producing fluorinated GHGs (for example, HFCs, PFCs, SF_6, NF_3, and fluoroethers), but also from processes and facilities producing fluoropolymers, which are often produced using HCFC, HFC, PFC, and other fluorochemical feedstocks. For some inventory compilers, identifying smaller producers and, in particular, recycling firms may be a difficult task. However, initial estimates based on the national mass balance of these fluorinated greenhouse gases should identify if production related emissions from such entities provide a sizeable contribution to total national emissions.

DEVELOPING A CONSISTENT TIME SERIES

Both by-product and fugitive emissions of fluorocompounds from production processes should be estimated using the same method for the entire time series and appropriate emission factors. If data for any years in the time series are unavailable for the Tier 3 method, these gaps should be filled according to the guidance provided in Volume 1, Chapter 5.

3.10.2.3 UNCERTAINTY ASSESSMENT

Uncertainty related to use of the Tier 1 default emission factors includes the uncertainty in the activity data and the assumptions made in estimating the destruction efficiency used in the uncontrolled emissions analysis. For Tier 1, the uncertainty in activity data needs to be determined for the reporting country and statistically combined with the uncertainty in the default emission factor. Typically, in a well operated facility, the default uncertainty in activity data should be in the region of 1 percent, assuming that rigorous accounting records are maintained and that production is monitored by weight. There are numerous sources of uncertainty in the default Tier 1 emission factor. One is the uncertainty associated with the fact that true uncontrolled emission rates naturally vary from facility to facility depending on the fluorochemicals produced and the processes used to make them. This variability appears in the US EPA data as differences in the calculated uncontrolled emission factors across facilities, differences that persist over the entire time series. The year-to-year variability seen in the calculated uncontrolled emission factor for any one facility is generally much smaller than this facility-to-facility variability. The uncertainty shown in Table 3.28a for the default EF for any other fluorochemicals reflects this variation among facilities. The 95 percent confidence interval (calculated based on the relative standard deviation among the facilities' emission factors) is ±470 percent. Because there cannot be a negative emission factor on the low side, a value of 0.001 was selected as the lower uncertainty bound, as it is representative of lower emission factor values seen in the data set. This results in an uncertainty range for the Tier 1 default emission factor of 0.001 to 0.2.

Another source of uncertainty for the default EF for any other fluorochemicals is the exact extent to which the emissions from individual processes are controlled by the facilities reporting to the US EPA GHGRP. As noted above, the level of abatement (destruction efficiency, or DE) is reported as a range rather than a point estimate, but a point estimate must be used to back-calculate uncontrolled emissions. Thus, there is uncertainty in the choice of this point estimate and in the uncontrolled emissions used to calculate emission factors for each facility and year. In addition, there is uncertainty regarding the exact mix of fluorinated GHGs that would be emitted from each process without controls. Emissions at the facility level are generally reported by chemical, but emissions at the process level are reported by chemical group. While this provides general process-level information on the nature and GWP of the emitted GHGs, the GHGs that fall into each group vary in their GWPs.

However, both of these sources of uncertainty are mitigated by the large number of data points in the analysis, which come from the large number of processes and significant number of years covered. Thus, the errors related to the destruction efficiency estimated for each individual process and to the mix of gases emitted tend to balance out, and the aggregate uncertainty is reduced. A Monte Carlo analysis indicated that the uncertainty for each facility's uncontrolled emission factor was less than 50 percent.

For Tier 3 emissions, the uncertainty of the measurements should be determined individually and combined (using standard statistical methods) to provide a total uncertainty for the estimate. The methodology is identical to that described for HFC-23 from HCFC-22. In the Tier 2 methodology, the uncertainty both of the measurements of efficiencies and the assignment of losses to individual compounds should be assessed. Because these are liable to produce a much larger uncertainty than that from Tier 3, the utility of Tier 2 is likely to be limited to assessing whether or not by-product fluorochemical emissions are a significant subcategory under *key category*.

3.10.2.4 QUALITY ASSURANCE/QUALITY CONTROL (QA/QC), REPORTING AND DOCUMENTATION

No Refinement

3.11 HYDROGEN PRODUCTION

Hydrogen (H_2) is a gas with flammable properties similar to natural gas and gasoline (Hydrogen Council, 2017). The main current uses of hydrogen are as raw material in refineries and in the production of ammonia, methanol and other chemicals. Other uses are as an energy carrier in the transport sector, as energy storage and buffer systems in renewable electricity production, as a main constituent in coal gas (city gas) used for heating and cooking, as well as in semiconductor industry processing and welding. Production of hydrogen may yield emissions of carbon dioxide (CO_2), depending on the production method, while combustion or conversion of hydrogen to produce heat and electricity yields zero carbon dioxide emissions. An increase in the production, storage and use of hydrogen is expected in the future, due to an increased demand for low-carbon fuels and technologies.

3.11.1 Introduction

This section describes methodological guidance for estimating emissions from Hydrogen production. The methods are primarily applicable to instances where hydrogen is produced as the main product at a stand-alone facility. Note that where hydrogen is produced as part of a gas mixture (for instance in the case of syngas production – see Box 3.19), or as a by-product or intermediate product within another chemical or petrochemical process, then the GHG emissions should be estimated using methods for the most appropriate main product. For example, hydrogen is commonly produced as a by-product or intermediate product at petroleum refineries and at chemical facilities producing ammonia, methanol, and other products. In these instances, it is *good practice* for inventory compilers to apply the methodological guidance specific to those processes, as provided elsewhere within Volume 2 (Energy) and Volume 3 (IPPU), including:

- Volume 2, section 4.2 Fugitive emissions from oil and natural gas systems (includes guidance for emissions from hydrogen production in petroleum refineries, with resultant GHG emissions to be reported under 1.B.2.a.i);
- Volume 3, section 3.2 Ammonia production (with resultant GHG emissions to be reported under 2.B.1);
- Volume 3, section 3.9 Petrochemical and carbon black production (includes guidance for production of methanol and ethylene, both of which may also generate hydrogen by-product, with resultant GHG emissions to be reported under the appropriate sub-sector(s) of 2.B.8).

Hydrogen Production Technologies

Hydrogen can be produced through a wide range of chemical, thermochemical and biological processes; Table 3.29 below presents an overview of the current status (in terms of scale of production) and associated GHG emissions of each known technology.

The predominant hydrogen production technologies, accounting for more than 95 percent of global hydrogen production, are steam reforming and gasification of fossil fuels (Ogden, 1999; Speirs *et al*., 2017). Steam reforming and gasification are thermochemical technologies using feedstock from fossil or renewable sources, which is combined with heat and catalysts to trigger chemical reactions for transforming the feedstock (for example, natural gas, LPG, naphtha, coal, methanol, biomass and waste) into a gas mixture rich in hydrogen. When hydrogen is the final product (see Box 3.15), a series of enhancement and purification steps yields a highly pure hydrogen output (99.95 percent purity is typical at present).

Production of hydrogen by water electrolysis is widespread, mainly in small-scale plants, and accounts for about 4 percent of current global hydrogen production. Other methods for hydrogen production are currently at a minor or experimental level. Several of the production methods, e.g. water electrolysis and photo induced water splitting, do not generate direct GHG emissions from the hydrogen production process. Others, e.g. steam reforming of ammonia and thermal water splitting, generate no *process* emissions of GHGs but do emit GHGs from stationary *combustion of fuels* to heat the production process, and accordingly these emissions should be reported in the Energy sector.

Biological methods to generate hydrogen are currently at a very small-scale, and typically involve a fermentation process to produce hydrogen, using living microbes such as algae and bacteria. In the production process either fossil or biogenic materials are consumed under anaerobic conditions, and the output products are hydrogen gas containing minor amounts of CO_2, CH_4 and other organic substances, and CO_2 off-gas which may be partly captured by the microbes; at present a maximum of 2 percent CH_4 by mass in the hydrogen product is reported in some anaerobic biological methods (Braga et al 2017). Any CH_4 and CO_2 produced in the process will become a constituent part of the fermentation gas product, and any subsequent emissions from this gas use should be reported in the sector(s) where it is used. Hence, emissions from hydrogen production by biological methods are considered negligible and should not be reported in the hydrogen production sector.

Further development and increased uptake of low-emission hydrogen production methods is anticipated, however, methods using fossil feedstock currently dominate due to economic reasons (Speirs *et al*., 2017).

Hydrogen Production: GHG Emission Sources and Reporting Allocations

There are many different hydrogen production technologies, and their contribution to GHG emissions range from zero direct emissions at the production facility (e.g. water electrolysis) to significant direct GHG emissions (e.g. from steam reforming or gasification of fossil feedstocks). Of the directly emissive technologies, some utilise fossil fuels only *for combustion*, to heat the process, with no *chemical process* GHG emissions associated with the hydrogen production, such as dehydrogenation or thermal water splitting, whilst hydrogen production through steam reforming or gasification of fossil materials does result in both *chemical process* and *combustion*-derived GHG emissions.

Table 3.29 provides information on *best practice* for the reporting allocation of emissions from each technology, and further guidance is as follows:

(i) The GHG emissions from hydrogen production as a pure main product at a stand-alone facility should be reported under the Hydrogen production sector in IPPU. This typically includes GHG emissions from hydrogen production technologies that generate process emissions from fossil feedstocks, i.e. steam reforming or gasification of fossil materials. Hydrogen production methods that generate no direct GHG emissions, such as the electrolysis of water, should not be considered in the IPPU sector;

(ii) It is *good practice* to report under Hydrogen Production all the GHG emissions from steam reforming and gasification of fossil materials, including the *fuel combustion* and *chemical process* emissions from the fuels and feedstock, and to exclude these fuel combustion emissions from the Energy sector, in line with the IPCC methods for other similar chemical processes, such as production of ammonia (2B1) and petrochemicals (2B8).

(iii) Emissions of CO_2 from thermochemical processes such as steam reforming and gasification using *biomass* as feedstock should be reported as a memo item only, to avoid double counting with emissions reported in source categories in Agriculture, Forestry and Other Land Use (AFOLU). If the feedstock contains both fossil and biogenic components (e.g., auto diesel mixed in with biodiesel, waste, etc.), the CO_2 emission should be allocated partly to the Hydrogen production sector and partly to the memo item, relative to the respective fossil and biogenic carbon shares.

(iv) As noted above, where hydrogen is produced as a by-product for sale or as an intermediate product in a source category provided with methodological guidance on GHG emissions from hydrogen production, it is *good practice* to estimate GHG emissions by applying the methodological guidance for the appropriate source category. These source categories include:

   a. Petroleum refineries (Volume 2, section 4.2)

   b. Ammonia production (Volume 3, section 3.2)

   c. Methanol production and ethylene production (Volume 3, section 3.9)

(v) Where GHG emissions arise from production of intermediate or by-product hydrogen (including gas mixtures containing hydrogen) in sectors *not* provided with a methodology for estimating these emissions, it is *good practice* to use one of the methodological approaches provided in Volume 3 IPPU (ammonia, methanol or hydrogen), as follows:

   a. If the feedstock is completely oxidized and the main product does not contain carbon, the methodology for hydrogen production should be used.

   b. If the feedstock is partly oxidized and the main product does not contain carbon, the methodology for ammonia production should be used.

   c. If the main product contains carbon, the methodology for methanol production and ethylene production should be used.

The compiler should use the methodology that minimises uncertainties in the national inventory, transparently note which method(s) are used, and report the GHG emissions in the appropriate source category of the main product for that facility.

(vi) Where hydrogen is produced as part of a hydrogen carrier, or released from such a hydrogen carrier system, the GHG emissions yielded from the process may be allocated to a range of different sectors, according to the carrier type. See Box 3.17 for further details.

(vii) Where activity data for hydrogen production at the national level may combine data from stand-alone facilities and integrated facilities within other sectors, and from emissive and non-emissive technologies, inventory compilers should take care to ensure that gaps and double counting of emissions do not occur.

In light of the range of production technologies, it may be difficult for inventory compilers to obtain fully-resolved activity data by technology, making it difficult to estimate and report GHG emissions consistent with the good practice methods outlined above.

As for all inventory source categories, it is *good practice* to estimate and report emissions from hydrogen production such that inventory uncertainties are minimised, and to minimise the risk of any gaps or double-counts in the reported estimates across Energy and IPPU source categories. In the event that the good practice approach to reporting hydrogen production cannot be achieved due to national circumstances, then inventory compilers should transparently document the methods applied, note where emissions from hydrogen production are included (fully or in part) within Energy and/or other IPPU source categories, and derive uncertainty estimates that reflect the country-specific approach.

See Box 3.16 for details about double counting.

Reporting of GHGs contained within the hydrogen product

Some hydrogen production methods generate GHGs as an unintended constituent of the product. For instance, hydrogen produced by biological processes may contain minor amounts of methane. In these cases, the GHGs are emitted after the product has been sold to an end user, either from the use or fugitive release of the product itself or from the combustion of it. It is *good practice* to estimate GHG emissions using methods specific to the final emission source, and report the emissions in that sector, and not in the Hydrogen production sector.

Carbon Dioxide Capture and Storage

Should CO_2 capture technology be installed and used at a plant where hydrogen is produced from steam reforming or gasification of fossil materials, it is *good practice* to deduct the CO_2 captured in a higher tier emissions calculation. The default assumption is that there is no CO_2 capture and storage (CCS). In most cases, methodologies that account for CO_2 capture should consider that CO_2 emissions captured in the process may be both combustion and process-related. However, in the case of hydrogen production from steam reforming or gasification of fossil materials, no distinction is made between fuel and feedstock emissions with all emissions accounted for in the IPPU Sector. Similarly, all CO_2 captured should be accounted for in the IPPU Sector. For additional information on CO_2 capture and storage, refer to Volume 3, Section 1.2.2 and for more details on capture and storage to Volume 2, Section 2.3.4.

CH_4 and N_2O emissions from hydrogen production

Steam reforming and gasification produce very minor emissions of CH_4 and N_2O, in addition to CO_2 emissions. The available literature indicates that emissions of CH_4 and N_2O are very low, activity data for the process combustion source are likely to be hard to obtain, and the literature evidence is insufficient to establish an estimation method. Hence, no reporting of CH_4 and N_2O is required in this sector.

BOX 3.15 (NEW)
DEFINITIONS

Pure hydrogen and gas mixtures

Pure hydrogen is hydrogen gas that has been purified to meet industry product quality standards. Pure hydrogen is produced by *complete oxidation* of feedstocks or by other technologies (Table 3.29).

Hydrogen that is produced by technologies that *partially oxidize* a hydrocarbon feedstock will also contain other gases (typically CH_4, CO, CO_2, other hydrocarbons) and is defined as a "gas mixture".

Final products and intermediate products

A final product is an intended output product from a production facility. The final product can be either sold as a commercial product or exported offsite for use in another facility. An intermediate product is an output from one production process, which is consumed as raw material or fuel in a later production step at the same facility.

Main products and by-products

A main product is the product defining a facility's sector in the IPCC reporting. As a rule of thumb, the main product is the product generating the highest monetary production value. By-products are all other products made intentionally at the facility. If nothing else is stated, main products and by-products are final products.

Feedstock, raw material and fuel

In this section, feedstock means the total input material in a manufacturing process. Raw material is the part of the feedstock being transformed into the final or intermediate product(s). Fuel is a material combusted to produce heat. The fuel might be derived from the feedstock (i.e. internal energy source) or provided separately (i.e. external energy source).

TABLE 3.29 (NEW)
CURRENT HYDROGEN PRODUCTION METHODS – STATUS OF DEVELOPMENT AND ALLOCATION OF EMISSIONS TO SECTOR

Category	Technology	Feedstock	Status of development[1]	Sector	Allocation principle
Pure main product hydrogen	Steam reforming	Fossil	Major	Hydrogen production[2]	Fossil process emissions
		Biofuel	Minor	Memo	Biogenic process emissions
		Waste	Minor and increasing	Hydrogen production[2] /Memo	Fossil/biogenic[3] process emissions
		Methanol	Minor and mature	Hydrogen production[2]	Fossil process emissions
	Gasification	Fossil	Major	Hydrogen production[2]	Fossil process emissions
		Biomass	Minor	Memo	Biogenic process emissions
		Waste	Minor and increasing	Hydrogen production[2] /Memo	Fossil/biogenic[3] process emissions
	Water electrolysis	Water	Moderate and increasing	Not applicable	No direct emissions[5]
	Dehydrogenation	Organic Hydride[6]	Minor	Energy (stationary combustion)	Only combustion emissions
		Ammonia	Minor	Energy (stationary combustion)	Only combustion emissions[4]
	Fermentation	Biomass	Experimental	Not applicable	No direct emissions[5]
	Methane cracking	Natural gas	Minor	Energy (stationary combustion)	Only combustion emissions[4]
	Thermal water splitting	Water	Experimental	Energy (stationary combustion)	Only combustion emissions[4]
	Photo catalytic splitting	Water	Experimental	Not applicable	No direct emissions[5]
	Photo biological splitting	Water	Experimental	Not applicable	No direct emissions[5]
By-product or intermediate product hydrogen[2]	Refining of crude petroleum	All	Major	Energy (fugitive)	Hydrogen produced as by-product or intermediate product
	Ammonia production	All	Major	Ammonia production	Hydrogen produced as by-product or intermediate product
	Methanol production	All	Major	Petrochemical and Carbon Black	Hydrogen produced as by-product or intermediate product
	Ethylene production	All	Minor	Petrochemical and Carbon Black	Hydrogen produced as by-product or intermediate product
	Steel production	All	Minor	Iron and Steel and Metallurgical Coke	Hydrogen produced as by-product or intermediate product
	Caustic soda production	Sodium chloride	Moderate	Not applicable	Produced by electrolysis. No direct emissions[5]
	Fuel cell reforming	Methanol	Experimental	Sector of the end user	Hydrogen produced as an intermediate product
		Fossil	Minor and increasing	Sector of the end user	Hydrogen produced as an intermediate product

TABLE 3.29 (NEW) (CONTINUED)
CURRENT HYDROGEN PRODUCTION METHODS – STATUS OF DEVELOPMENT AND ALLOCATION OF EMISSIONS TO SECTOR

Notes:

[1] Status of development refers to the current situation in a global scale. Major, moderate and minor reflect the amount of industrial hydrogen production. Experimental means that the hydrogen is not yet produced in an industrial scale.

[2] Where hydrogen is produced as a by-product or intermediate product, the emissions are typically already accounted for in the emission estimates for the respective sectors derived using methodological guidance in Volume 3 Energy or Volume 4 IPPU. Emissions from production of hydrogen as part of mixtures with other gases, e.g., syngas, are not covered by this section. See Box 3.15 for the definition of main product, by-product and intermediate product and Box 3.16 about double counting.

[3] Non-biogenic emissions are reported to IPPU and biogenic emissions are reported as a memo item (i.e. not included in the IPPU totals).

[4] No process emissions, as the feedstock does not contain carbon. All emissions arise from combustion of fuels to power the production process.

[5] Only direct emissions (i.e. emissions generated in the production facilities during production) are considered, according to standard IPPU methodology.

[6] In dehydrogenation, the raw material is not consumed. Hence, all emissions come from fuel combusted to produce heat for the reaction.

BOX 3.16 (NEW)
DOUBLE COUNTING, COMPLETENESS AND CROSS-CUTTING ALLOCATION

- In order to avoid double counting, activity data and emissions from production of hydrogen reported in the **Hydrogen production sector** must be excluded from other sectors, i.e. the total quantities of oil, gas, coal and other fossil materials (fuel plus feedstock) used in hydrogen production must be subtracted from the quantity reported under energy use in the Energy sector. Conversely, activity data and emissions from production of hydrogen reported in the **Energy sector** and **IPPU sectors other than Hydrogen production** must be excluded from the Hydrogen production sector.

- Where the level of activity data resolution does not enable separation of the production of hydrogen as a pure product, by-product or gas mixture, then it is *good practice* for compilers to calculate and report emission estimates such that (i) the emission estimates are complete with no double-counting, and (ii) that overall inventory uncertainty is minimised. Further, it is *good practice* to clearly explain the national circumstances, activity data, methods and reporting allocations in inventory submissions.

- In many hydrogen production processes, the same fossil material is used both as raw material for the production process and as fuel combusted to heat the process. It is impractical to seek to distinguish between “fuel” and “feedstock” and to report these emissions separately. Therefore, it is *good practice* to report both the fuel combustion and chemical process emissions in the Hydrogen production sector, and to exclude these fuel combustion emissions from the Energy sector, consistent with the IPPU cross-cutting guidance as presented in Vol. 3 IPPU, Chapter 1.2.1 and Box 1.1.

- To minimise the risk of gaps and double-counts, inventory compilers may need to consult with statistical agencies, trade associations and plant operators as appropriate, to seek to ensure that the hydrogen production activity data does not include any hydrogen derived from non-emissive technologies, nor any production of hydrogen as a by-product or intermediate within facilities that produce other main outputs such as refineries, ammonia and methanol plant where the GHG emissions are already accounted for elsewhere in the inventory.

- Recovered CO_2 might be delivered for downstream use, for instance as raw material in other manufacturing processes or as dry ice (cooling, cleaning, etc.), or sent to a permanent storage. When used in a downstream manufacturing sector, the CO_2 might be embedded into a product (for instance through a chemical reaction) or emitted to the atmosphere. It is *good practice* to report the emission of CO_2 from downstream use in the **downstream IPPU or other sector**, and to subtract the recovered CO_2 from the Hydrogen production sector.

- The downstream use and permanent storage of recovered CO_2 should be transparently described and must be documented in accordance with IPCC Guidelines. It is *good practice* to cross-check that all emissions from downstream use of recovered CO_2 is accounted for in the corresponding downstream sector(s).

BOX 3.17 (NEW)
PRODUCTION AND USE OF HYDROGEN CARRIERS

Hydrogen is a highly volatile gas, which may be transported through a pipeline or in tanks as a compressed gas or as a cryogenic liquid. To facilitate the safe, efficient transport and storage of hydrogen, a carrier chemical may be used. A ‘hydrogen carrier’ is a chemical substance containing hydrogen that is easy to store and transport, from which the hydrogen gas can be extracted through a chemical reaction for use in a downstream sector. Some carriers are recycled for subsequent hydrogen deliveries, while others are consumed in the process where the hydrogen is released.

Some hydrogen carriers are produced with a full load of hydrogen in a single-step process. Other hydrogen carriers are produced and loaded with hydrogen in a two-step process, first as an “empty” carrier. Subsequently, the hydrogen (normally produced at a different plant) is embedded into the empty carrier through a chemical reaction.

The hydrogen carrier is transported to a downstream facility, for example a refuelling station, where the hydrogen is released by a chemical reaction (dehydrogenation) and filled into a vehicle or machine, or the hydrogen carrier itself is filled into a fuel cell, in which the hydrogen (H_2) is released and consumed.

The different types of hydrogen carrier chemicals have the GHG emissions from their production and use allocated to different sectors.

Organic hydrides

Hydrogen can be reacted with aromatic substances such as benzene and toluene to form liquid organic hydrides.

The emissions from the manufacturing of hydrogen should be allocated to the *Hydrogen production* sector, while the emissions from production of the aromatic substances used as “empty carriers” should be allocated to the *Petrochemical and carbon black* sector.

The reaction releasing hydrogen at the downstream facility produces no process emissions of GHGs. Instead, the organic hydride is converted back to the original aromatic substance and transported to the hydrogen production facility to embed more hydrogen, in a circular material flow pattern. The hydrogen-releasing reaction requires heat, which might be produced by combustion of fossil fuels. In such cases, the emitted CO_2 should be allocated to the Energy sector (stationary combustion).

Ammonia

Ammonia (NH_3) is a hydrogen-rich gas that can be cooled down and/or compressed into a liquid and transported to a downstream facility or fuel cell. There the hydrogen (H_2) may be released by a chemical reaction (dehydrogenation).

The emissions from the ammonia production process should be allocated to the *Ammonia production* sector, even though the purpose of producing the ammonia is to derive hydrogen for downstream use.

For the use of ammonia as hydrogen carrier, no emissions should be allocated to the *Hydrogen production* sector. The reaction releasing hydrogen at a downstream facility produces no process emissions of CO_2, since the ammonia contains no carbon. Fossil combustion emissions from the hydrogen releasing reaction should be allocated to the Energy sector (stationary combustion).

Methanol

Methanol (CH_3OH) is a hydrogen-rich liquid that can be transported to a downstream facility, where the hydrogen may be released by a chemical reaction (e.g. steam reforming).

The emissions from the methanol production should be allocated to the *Petrochemical and carbon black* production sector, even though the purpose of producing the methanol is to derive hydrogen for downstream use.

The process at the downstream facility to release hydrogen from the methanol generates process emissions of CO_2. These emissions should be reported in the *Hydrogen production* sector, using the estimation methods provided for this sector.

Consumption of methanol in direct methanol fuel cells yields CO_2 emissions, but hydrogen (H_2) isn’t involved in the reactions. Accordingly, these CO_2 emissions should be reported in the Energy sector.

3.11.2 Methodological issues

The predominant methods for hydrogen production at present are steam reforming and gasification of fossil feedstocks. Both technologies oxidise the feedstock during the process itself and also in combustion to heat the process, releasing CO_2.

Technologies for producing hydrogen from fossil or biogenic feedstocks in an open, aerobic environment can be placed in either of two categories, according to the degree of conversion of the *feedstock carbon*: complete oxidation technologies and partial oxidation technologies.

Complete oxidation technologies convert all feedstock carbon into CO_2 (except for a small residue of solid carbon), and they have hydrogen as the main product. The CO_2 emissions can be estimated from feedstock consumption or hydrogen production data.

Partial oxidation technologies convert parts of feedstock carbon into CO_2, and they result in gas mixtures having hydrogen as a constituent. In several industries using hydrogen as a raw material, partial oxidation technologies[5] are often used to produce an intermediate mixture of hydrogen and CO (e.g. syngas production, see Box 3.19), as also CO is needed for raw material. To regulate the H_2:CO ratio, hydrogen might be separated from the mixture as a by-product and burnt for fuel or used externally (e.g. sold for use in a downstream sector).

A list of production methods and allocation by sector is given in Table 3.29.

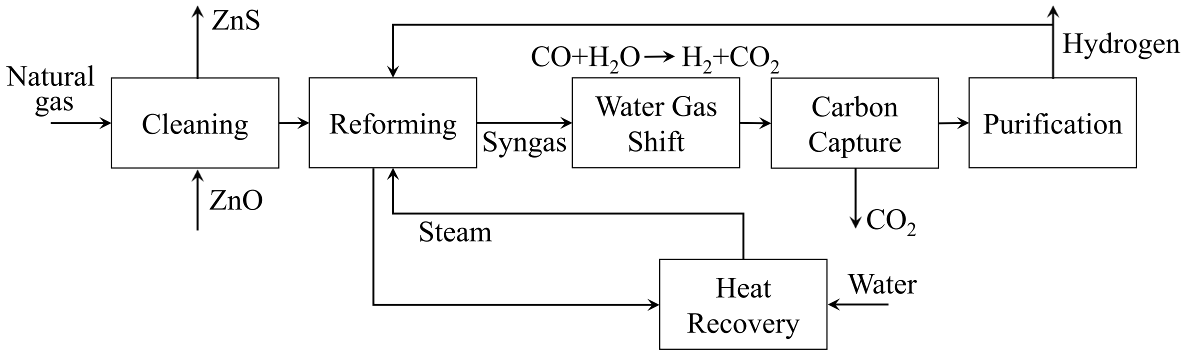
COMPLETE OXIDATION TECHNOLOGIES

The main complete oxidation technologies are steam reforming of natural gas and fossil liquids (Figure 3.18) and gasification of coal and lignite (Figure 3.19). Both production processes have several steps, in order to maximise the hydrogen output. The first one partially oxidizes the feedstock carbon and generates a gas mixture containing hydrogen, carbon monoxide and, in the case of gasification of coal and lignite, solid carbon. The next step further oxidizes the carbon by a water gas shift reaction, yielding even more hydrogen. An integrated combustion reaction using feedstock (or gasified feedstock) as fuel, or in some cases a support fuel, provides energy to produce steam for the water gas shift reaction.

Other feedstocks are sometimes used as well, though in a very small scale at present. The feedstock material may be fossil carbon in origin, biogenic carbon in origin, or a mixture of fossil and biogenic (such as the use of mixed wastes as a feedstock), but the underlying chemistry to derive the hydrogen is the same and hence the GHG emission estimation methods are similar.

In both the hydrogen producing (overall) reaction and the combustion reaction there is a close to 1:1 molar relation between the produced CO_2 and the carbon contained in the feedstock. The only exception is a small amount of solid carbon residue disposed of as waste.

Figure 3.18 (New) Hydrogen production via steam reforming with water gas shift reaction



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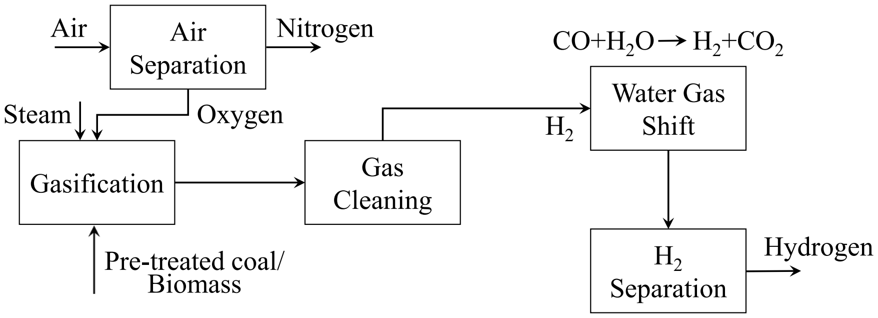
[5] Partial oxidation technologies include all technologies partially oxidizing the feedstock. One of these is commonly called "partial oxidation".

Figure 3.19 (New) Hydrogen production via gasification with water gas shift reaction[1]



Note:

[1] The flue gas from the H_2 separation step, containing CO and methane, is combusted in a boiler to produce heat (i.e. steam).

Source:

Matzen *et al*., 2015; The National Energy Technology Laboratory, 2017.

BOX 3.18 (NEW)

CHEMICAL REACTIONS IN HYDROGEN PRODUCTION BY COMPLETE OXIDATION TECHNOLOGIES

Steam reforming of natural gas (overall reactions):

1a) Reforming: $CH_4 + 2H_2O \rightarrow CO_2 + 4H_2$

1b) Combustion: $CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$

Steam reforming or gasification of other fossil or biogenic feedstocks (overall general formulas):

2a) Reforming or gasification: $C_aH_bO_c + (2a\text{-}c)*H_2O \rightarrow a*CO_2 + (2a+0.5b\text{-}c)*H_2$

2b) Combustion: $C_aH_bO_c + (a+0.25b\text{-}0.5c)*O_2 \rightarrow a*CO_2 + 0.5b*H_2O$

Gasification of waste (overall general formulas):

3a) Gasification:

$C_aH_bO_cN_dS_e + (2a\text{-}c+2d+2e)*H_2O \rightarrow a*CO_2 + d*NO_2 + e*SO_2 + (2a+0.5b\text{-} c+2d+2e)*H_2$

3b) Combustion:

$C_aH_bO_cN_dS_e + (a+0.25b\text{-}0.5c+d+e)*O_2 \rightarrow a*CO_2 + d*NO_2 + e*SO_2 + 0.5b*H_2O$

In all these overall reactions the ratio of consumed feedstock carbon atoms to produced CO_2 molecules is 1:1. The molar relation between each reforming or gasification reaction and the subsequent combustion reaction depends on the efficiency of the production process, and the ratio of produced hydrogen to produced CO_2 varies accordingly (Braga *et al*., 2017; Trane *et al*., 2012).

PARTIAL OXIDATION TECHNOLOGIES

Partial oxidation technologies are reforming and gasification technologies producing hydrogen and carbon monoxide (CO) in closed systems with a sub-stoichiometric supply of oxygen. The process typically includes the first reaction step in a complete oxidation technology producing a mixture of hydrogen and CO, and it might include one or more subsequent steps (e.g., a water gas shift reaction) to obtain the desired ratios for the two gases. Purified gases, including H_2, may be produced as a by-product.

Emissions from technologies partially oxidizing the feedstock, including syngas production (see Box 3.19 below), are not covered by the estimation methods in this section, to avoid double counting with other sectors.

BOX 3.19 (NEW)
SYNGAS

Syngas is a gas mixture containing hydrogen, carbon monoxide and sometimes smaller amounts of CO_2, methane and other gases as well. The hydrogen to carbon monoxide molar ratio varies from about 0.5 to 5 depending on the feedstock. Syngas is produced by different technologies partially oxidizing the feedstock, including steam reforming, gasification, partial oxidation and auto-thermal reforming, in the presence of heat. The feedstock may be natural gas, coal, liquid refinery residues or other carbon containing materials.

Syngas is typically used as an intermediate product in refineries, ammonia, methanol or other chemical industries, but production for offsite use as an energy product or separated into its single gases also occurs. Surplus hydrogen might be separated from the syngas and purified into a by-product to obtain a specific H:CO ratio in the syngas for use in the production process of the main product. Emissions from syngas production are not covered by the estimation methods in this section. Methods to estimate GHG emissions from syngas intermediate and hydrogen by-product production in petroleum refineries, ammonia, methanol and other chemical production are provided in the respective Energy and IPPU sectors.

Source:
Abbas, 2018; Copeland *et al*., 2005; Maurstad, 2005; The Global Syngas Technologies Council, 2018; The National Energy Technology Laboratory, 2018, 2002.

OTHER PRODUCTION METHODS

Biological methods including fermentation produce hydrogen by using living microbes like algae and bacteria. In the production process either fossil or biogenic raw materials are consumed under anaerobic conditions, and the output products are hydrogen containing minor amounts of CO_2, methane and other organic substances, and CO_2 off-gas. Methane and other GHGs being produced along with the hydrogen are parts of the product and should be reported in the sector(s) where it is used. The CO_2 off-gas is assumed balanced by the CO_2 taken up by the microbes, and should not be reported.

Production of hydrogen by other technologies than those mentioned above, including water electrolysis, photo induced water splitting, steam reforming of ammonia and thermal water splitting, are typically without process GHG emissions, and emissions from these production methods should not be reported in the Hydrogen production sector.

3.11.2.1 CHOICE OF METHOD

The choice of method will depend on the availability of activity data, as shown in the decision tree (Figure 3.20). The Tier 1c, 2c and 3c methods are based on feedstock consumption data, while the Tier 1b, 2b and 3b methods are based on hydrogen production data. The Tier 1a method is based on hydrogen production data on a total national or regional level, or hydrogen production capacity if production data are not available. There is no Tier method labelled 2a or 3a on this section.

If all relevant activity data are available, it is *good practice* to choose the method having the lowest overall uncertainty. A higher Tier method has a lower uncertainty than a lower one, and the Tier *c* method normally has a lower uncertainty than the Tier *b* method at the same Tier level. The Tier 1a method has the highest uncertainty.

CO_2 released from hydrogen production may be recovered, either for capture and storage or for use in other downstream manufacturing industries. In all emission estimation methods, it is *good practice* to subtract recovered CO_2 from the estimated emissions in the Hydrogen production sector and to include the emissions in the respective downstream IPPU sector(s). If the recovered CO_2 is sent to permanent storage, it is *good practice* to subtract the recovered CO_2 from the Hydrogen production sector.

The estimation methods below are presented using energy units (GJ) for feedstock activity data, and mass units (tonne) for the hydrogen production data. Where these parameters are reported in different units at the national or facility level (e.g. volume, mass) then unit conversions consistent with national or facility data or IPCC defaults may be applied.

Guidance on how to allocate the GHG emissions to the correct sector is given in the previous section (3.11.1).

TIER 1 METHOD

The Tier 1 methods use *national or regional level activity data* together with *default factors* and data on recovered CO_2 to derive emissions. This method should be used if country-specific factors (Tier 2) or plant specific activity data and factors (Tier 3) are not available and hydrogen production is not a *key category*. The activity data are consumption of feedstock (Tier 1c) or production of hydrogen (Tier 1b and 1a). In the Tier 1c and 1b methods the activity data are split by type of feedstock, and feedstock specific factors in Table 3.30 should be used. In the Tier 1a method total national or regional activity data and the general default factors in Table 3.30 could be used.

The CO_2 emissions are estimated as follows:

EQUATION 3.44 (NEW)
CO_2 EMISSIONS FROM HYDROGEN PRODUCTION – TIER 1C

$$E_{co_2} = \sum_j (FC_j \bullet CCF_j \bullet {}^{44}\!/_{12}) - R_{co_2}$$

EQUATION 3.45 (NEW)
CO_2 EMISSIONS FROM HYDROGEN PRODUCTION – TIER 1B

$$E_{co_2} = \sum_j (HP_j \bullet FRF_j \bullet CCF_j \bullet {}^{44}\!/_{12}) - R_{co_2}$$

EQUATION 3.46 (NEW)
CO_2 EMISSIONS FROM HYDROGEN PRODUCTION – TIER 1A

$$E_{co_2} = HP \bullet FRF \bullet CCF \bullet {}^{44}\!/_{12} - R_{co_2}$$

Where:

E_{CO2} = emissions of CO_2, tonne

FC = feedstock consumption in production of pure hydrogen as main product, GJ

HP = pure hydrogen produced as main product, tonne

FRF = feedstock requirement per unit of output, GJ feedstock / tonne hydrogen produced

CCF = carbon content factor, tonne C / GJ feedstock

j (subscript) = feedstock *j*

R_{CO2} = CO_2 recovered, tonne

Aggregate feedstock consumption data (FC) or hydrogen production data (HP) from national statistics may be used in the Tier 1 methods. For feedstock data obtained in tonne, conversion to GJ can be done by using the default calorific values in the Ch. 1. Vol. 2 of *2006 IPCC Guidelines* [6]. If data on feedstock consumption or hydrogen production are not available, hydrogen production capacity data might be combined with a utilization factor to estimate the hydrogen production in the Tier 1a method. The selection of activity data should aim to minimise the risk of any gaps or double-counting (Box 3.16) with hydrogen production from non-emissive technologies, or from partial oxidation technologies and fuel combustion already included in other inventory estimates.

The feedstock requirement factor (FRF) converts the production of hydrogen into the corresponding consumption of feedstock. The default values are given in Table 3.30. The carbon content factor (CCF) converts the feedstock into carbon equivalents, while 44/12 converts the carbon into CO_2.

It is *good practice* to estimate of the fossil and biogenic emissions separately, based on the respective fossil and biogenic carbon shares, and to allocate the biogenic emissions to a memo item and exclude it from the Hydrogen production sector. If the biogenic part cannot be estimated, it is *good practice* to assume that all feedstock is fossil. If no data on recovered CO_2 could be obtained, it is *good practice* to assume that the recovery is zero.

If activity data and factors for all the Tier 1 methods are available, it is *good practice* to use the method giving the lowest uncertainty.

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[6] For plastic gasification the NCV value is given in the footnote to Table 3.30.

TIER 2 METHOD

The Tier 2 methods use *national or regional level activity data* together with *country-specific factors* and data on recovered CO_2 to derive emissions, and should be used when hydrogen production is a *key category* and plant-specific activity data are not available. The activity data used in the Tier 2 method must be split by type of feedstock. The CO_2 emissions are estimated as follows:

EQUATION 3.47 (NEW)
CO_2 EMISSIONS FROM HYDROGEN PRODUCTION – TIER 2C

$$E_{co_2} = \sum_j (FC_j \bullet CCF_j \bullet 44/12) - R_{co_2}$$

EQUATION 3.48 (NEW)
CO_2 EMISSIONS FROM HYDROGEN PRODUCTION – TIER 2B

$$E_{co_2} = \sum_j (HP_j \bullet FRF_j \bullet CCF_j \bullet 44/12) - R_{co_2}$$

Where:

E_{CO2} = emissions of CO_2, tonne

FC_j = feedstock consumption in production of pure hydrogen as main product, feedstock j, GJ

HP_j = pure hydrogen produced as main product, feedstock j, tonne

FRF_j = feedstock requirement per unit of output, feedstock j, GJ feedstock / tonne hydrogen produced

CCF_j = carbon content factor, feedstock j, tonne C / GJ feedstock

R_{CO2} = CO_2 recovered, tonne

The equations used in the Tier 2 methods are equal to those used in the Tier 1 method labelled the same letter, the only difference between the two Tier levels being that country-specific factors are needed at the Tier 2 level. Aggregate hydrogen production data (HP_j) or feedstock consumption data (FC_j) from national statistics may be used in the Tier 2 method. If activity data and factors for both Tier 2 methods are available, it is *good practice* to use the method giving the lowest uncertainty. It is *good practice* to use feedstock requirement factors (FRF_j) reflecting whether internal or external energy sources are used to heat the process. If no information on internal vs. external energy source is available, it is *good practice* to use FRF_js for internal energy sources and to note that the information is missing. Double counting with other sectors should be avoided (Box 3.16).

The FRF_j converts the production of hydrogen into the corresponding consumption of feedstock. The carbon content factor (CCF_j) converts the feedstock into carbon equivalents, while 44/12 converts the carbon into CO_2.

It is *good practice* to estimate of the fossil and biogenic emissions separately, and to allocate the biogenic emissions to a memo item and exclude it from the Hydrogen production sector. A fuel containing a fossil and a biogenic part should be split according to the respective fossil and biogenic carbon shares. If country-specific factors and/or an adequate split of the activity data by type of feedstock are not available and Hydrogen production is not a *key category*, it is *good practice* to use the Tier 1 method.

TIER 3 METHOD

The Tier 3 methods use *process- and plant-level activity data and factors* together with data on recovered CO_2 and stored amounts of solid carbon to derive emissions. The CO_2 emissions are estimated as follows:

EQUATION 3.49 (NEW)
CO_2 EMISSIONS FROM HYDROGEN PRODUCTION – TIER 3C

$$E_{co_2} = \sum_{j,n} (FC_{j,n} \bullet CCF_{j,n} \bullet 44/12) - (R_{co_2} + S_c \bullet 44/12)$$

EQUATION 3.50 (NEW)

CO_2 EMISSIONS FROM HYDROGEN PRODUCTION – TIER 3B

$$E_{co_2} = \sum_{i,j,n} (HP_{i,j,n} \bullet FRF_{i,j,n} \bullet CCF_{j,n} \bullet 44/12) - (R_{co_2} + S_c \bullet 44/12)$$

Where:

E_{CO2} = emissions of CO_2, tonne

$FC_{i,j.n}$ = feedstock consumption in production of pure hydrogen as main product, process i and feedstock j and plant n, GJ

$HP_{i,j,n}$ = pure hydrogen produced as main product, process i and feedstock j and plant n, tonne

$FRF_{i,j.n}$ = feedstock requirement per unit of output, process i and feedstock j and plant n, GJ feedstock / tonne hydrogen produced

$CCF_{i,j,n}$ = carbon content factor, process i and feedstock j and plant n, tonne C / GJ feedstock

R_{CO2} = CO_2 recovered, tonne

S_C = stored solid carbon, tonne

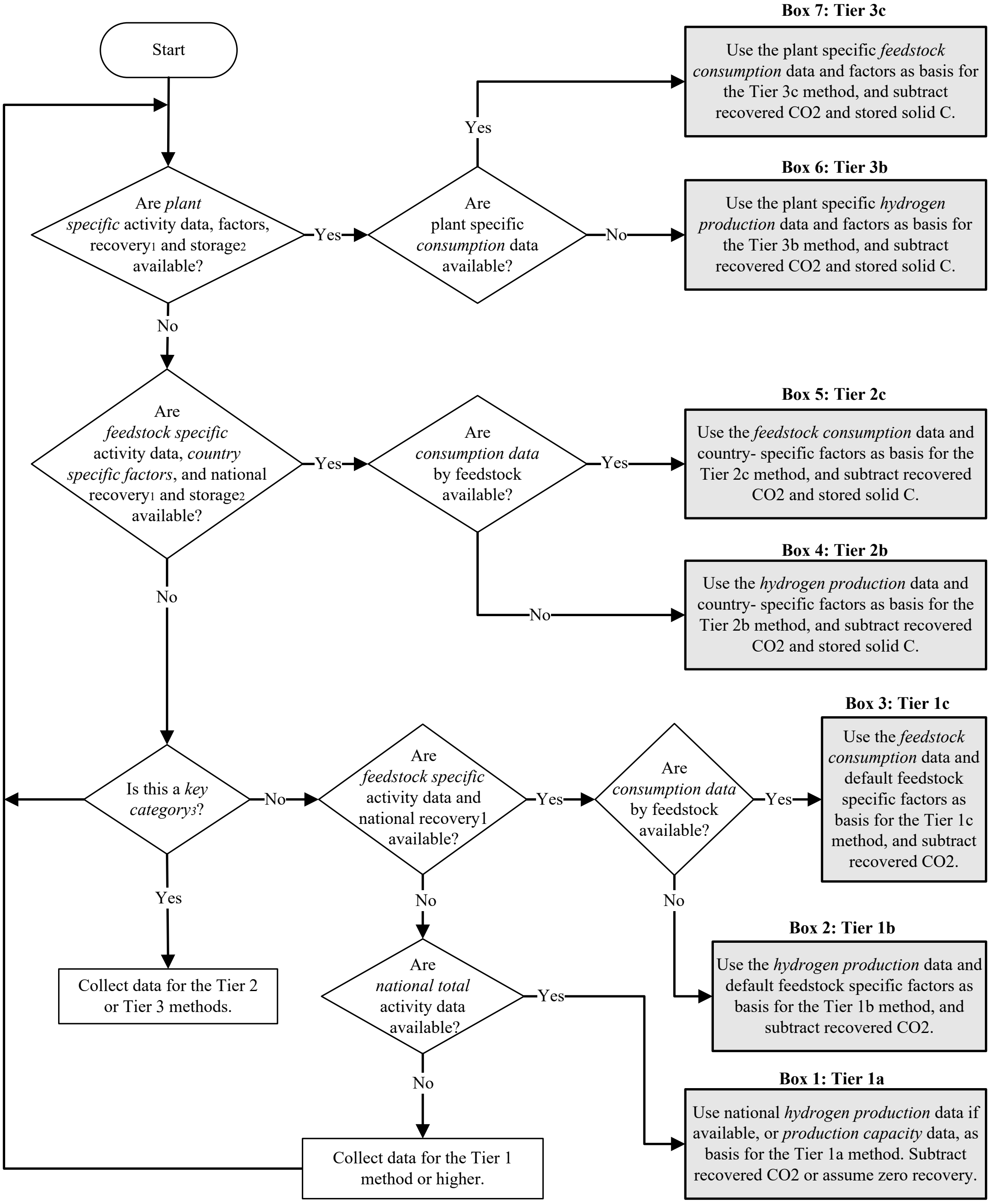
Plant, process and feedstock specific activity data and factors should be obtained from the hydrogen producers. Double counting with other sectors should be avoided (Box 3.16). If activity data and factors for both Tier 3 methods are available, it is *good practice* to use the method giving the lowest uncertainty.

The FRFs should take into account whether or not the fuel used to heat the process is derived from the feedstock (i.e. internal or external energy source). Emissions from fossil and biogenic fuels should be estimated separately, and the biogenic emissions should be allocated to a memo item and excluded from the Hydrogen production sector. Fuels containing a fossil and a biogenic part should be split according to the respective fossil and biogenic carbon shares.

Stored solid carbon here refers to solid carbon or coke formed unintentionally during the production process and disposed of as waste (i.e., not combusted at the production facility). Where no information on the carbon content in the stored solid carbon is available, it is *good practice* to assume that it is pure carbon. It is *good practice* to exclude stored solid carbon from the estimated emissions in the Hydrogen production sector. In the Hydrogen production sector, stored solid carbon does not include recovered CO_2 sent to permanent storage.

If plant, process and feedstock specific activity data and factors are not available and emissions from hydrogen production is a *key category*, it is *good practice* to use a Tier 2 method. If emissions from hydrogen production is not a *key category*, a Tier 1 method may be used.

Figure 3.20 (New) Decision tree for estimation of CO_2 emissions from hydrogen production



Note:

[1] Recovery = annual mass of CO_2 recovered from the hydrogen production emissions.

[2] Storage = annual mass of solid C generated in the hydrogen production emissions and disposed of as waste.

[3] See Volume 1 Chapter 4, Methodological Choice and Identification of *Key Categories* (noting Section 4.1.2 on limited resources), for *key categories* and use of decision trees.

3.11.2.2 CHOICE OF EMISSION FACTORS

The feedstock requirement factor (FRF) converts the production of hydrogen into the corresponding consumption of feedstock (raw material and fuel). The carbon content factor (CCF) converts the amount of feedstock in GJ into tonne of carbon.

TIER 1 METHOD

In the Tier 1c method, it is *good practice* to use the default feedstock specific CCFs in Table 3.30, and in the Tier 1b it is *good practice* to use the default feedstock specific FRFs and CCFs. These default values often represent midpoint or mean values of data sets (as determined by expert analysis). In the Tier 1a method, it is *good practice* to use the default FRF_j and CCF_j for the feedstock *j* giving the highest combined value (FRF_j * CCF_j) for the factors. This feedstock *j* should be among the commonly used feedstock types in the country, and the FRF_j and CCF_j should be used for the entire production. If no qualitative information on feedstock types is available, the general default factors might be used. The general default factors are weighted averages of the respective feedstock specific factors, based on global production figures.

TABLE 3.30 (NEW)
DEFAULT FEEDSTOCK REQUIREMENT FACTORS AND CARBON CONTENT FACTORS FOR HYDROGEN PRODUCTION[1,2]

Production Process	Feedstock Requirement Factor (FRF) (GJ feedstock/tonne H_2) ± Uncertainty[1]	Carbon Content Factor (CCF)[2] (tonne C / GJ feedstock)		
Steam reforming		**Default**	**Lower**	**Upper**
Natural gas reforming	165 (± 10%)	0.0153	0.0148	0.0159
Liquified petroleum gas reforming	165 (± 15%)	0.0172	0.0168	0.0179
Naphtha reforming	165 (± 15%)	0.0200	0.0189	0.0208
Methanol reforming	165 (± 20%)	0.0188	0.0186	0.0190
Biosteam reforming, other liquid (bioethanol)	175 (± 20%)	0.0217	0.0183	0.0260
Gasification				
Coal gasification (coking coal)[3]	215 (± 20%)	0.0258	0.0238	0.0276
Plastic[4] gasification	185 (± 10%)	0.0200	0.0160	0.0240
Mixed waste gasification (non-biomass fraction)	275 (± 15%)	0.0250	0.0200	0.0330
Wood waste gasification	260 (± 10%)	0.0305	0.0259	0.0360
Wood sludge gasification	195 (± 15%)	0.0305	0.0259	0.0360
Black liquor gasification	150 (± 10%)	0.0260	0.0220	0.0300
General				
Default	175 (± 30%)[5]	0.0183[6]	0.0148[6]	0.0276[6]

Notes:

1 When uncertainty range is not given in the referenced literature for a given factor, a default uncertainty of ±20% is chosen. When only one literature value is found, a default minimum uncertainty of ±15% is chosen.

2 The factors are also found in Table 1.3 Default values of carbon content in Volume 2.

3 Hydrogen production from coal is currently dominated by use of coking coal as feedstock. Where coal of other quality is used, then it is *good practice* in the Tier 1 method to: (i) apply the FRF for coking coal with an uncertainty range of ±30% when the Tier 1b method is used, and (ii) apply a default CCF that reflects the specific coal type (e.g. lignite, sub-bituminous, other bituminous) as presented in Table 1.3 of Volume 2.

4 Mixed plastic. For CCF the value for "other petroleum products" in Vol.2 Ch. 1 Table 1.3 is used. NCV = 32.0 MJ/kg.

5 Estimated by weighted average of natural gas (49%), LPG/naphtha (29%) and coal (18%), current production methods, based on global production statistics (remaining 4% is mainly produced by electrolysis of water). Uncertainty set to cover the ranges of these three feedstock types, which are by far the most common at present.

6 Estimated by weighted average of natural gas (49%), LPG/naphtha (29%) and coal (18%), current production methods, based on global production statistics (remaining 4% is mainly produced by electrolysis of water). Lower uncertainty range is from steam reforming of natural gas, upper uncertainty range is from gasification of coal.

Source:

Amgad *et al*., 2013; API, 2009; Cormos, 2011; DOE, 2017; Edwards *et al*., 2014; Geissler, *et al*., 2001; Iwasaki, 2003; JARI, 2011; Schiebahn *et al*., 2015; Sørensen, 2011; Themelis *et al*., 2011; The Pacific Northwest National Laboratory, 2017; US Department of Energy, 2017; Wallman *et al*., 1998.

TIER 2 METHOD

For the Tier 2c method it is *good practice* to use country-specific CCFs, and to quality check these factors against the default factors in Table 3.30.

For the Tier 2b method, it is *good practice* to use country-specific FRFs and CCFs, and to quality check these factors against the default factors in Table 3.30 to ensure good factor quality.

TIER 3 METHOD

Plant-level activity data on total fuel and feedstock requirement combined with CCF or hydrogen production combined with CCF and FRF by production technology and feedstock type provide the most rigorous data for calculating CO_2 emissions from hydrogen production. In the Tier 3 methods, it is *good practice* to use plant and feedstock specific CCFs, or plant, process and feedstock specific FRFs and CCFs, and to quality check these factors against the default factors in Table 3.30 to ensure good factor quality. The carbon content (CCF) is a key emission factor variable for deriving the quantity of CO_2 emissions in all Tier methods. Derivation of emissions using plant-level hydrogen production also depends on an accurate estimate of the fuel requirement per unit of output (FRF), along with information on the other variables.

3.11.2.3 CHOICE OF ACTIVITY DATA

For all methods, it is good practice to gather activity data on hydrogen production from national or regional data sources (e.g. statistical agencies, regulatory agencies, plant operators, trade associations, researchers) in order to minimise the risk of gaps and double-counting in the inventory (Box 3.16). Data on CO_2 recovered from hydrogen production (for use downstream, or to storage) should also be sought. It is *good practice* to use the Tier method giving the lowest overall uncertainty.

TIER 1 METHOD

National or regional level activity data may be used in the Tier 1 methods:

- In the Tier 1c method, *feedstock consumption data* by type of feedstock should be used;
- In the Tier 1b method, *hydrogen production data* by type of feedstock should be used;
- In the Tier 1a method, *total hydrogen production data* should be used.

If feedstock consumption or hydrogen production data are not available for the Tier 1c method, production capacity data may be used instead. If the inventory compiler can document that utilisation for a year was below capacity, it is *good practice* to multiply the total national or regional production capacity by a default capacity utilisation factor of 80 percent ± 10 percent (i.e., a range of 70-90 percent) through the entire time-series, or a country-specific capacity utilisation factor. If production capacity data are used for the base year and actual production data are used for later years, a country-specific capacity utilisation factor should be used for all years with production capacity data. It is *good practice* to estimate this capacity utilisation factor as the actual hydrogen production divided by the production capacity of at least one overlapping year adjacent to the years with production capacity data.

It is *good practice* to obtain the biogenic share of the feedstock, to estimate the CO_2 emissions to be excluded from the Hydrogen production sector and reported in a memo item. If the biogenic share cannot be obtained, it is *good practice* to assume that all feedstock is fossil.

Where feedstock data are obtained in tonnes, the default calorific values in Ch. 1, Vol. 2 of *2006 IPCC Guidelines* can be used to convert to energy units.

TIER 2 METHOD

The Tier 2 methods requires the same activity data as the Tier 1 method labelled with the same letter (i.e. the same sub-Tier). The biogenic share of the feedstock should be obtained from the producers, and the estimated biogenic CO_2 emissions should be excluded from the Hydrogen production sector and reported in a memo item.

TIER 3 METHOD

The Tier 3 methods require the collection of plant-level activity data by production method and type of feedstock, including plant-level data on recovered CO_2, where applicable. Production capacity data should not be used. The biogenic share of the feedstock should be obtained from the producers, to estimate the CO_2 emissions to be excluded from the Hydrogen production sector and reported in a memo item.

Where access to plant-level data may be limited due to confidentiality, then inventory compilers should refer to guidance presented in Volume 1, Chapter 2 *Approaches to Data Collection*.

3.11.2.4 COMPLETENESS

In countries where only a subset of plants report data for the Tier 3 method or where there is a transition from Tier 2 to Tier 3, it may not be possible to report according to Tier 3 for all facilities during the transition. Where data for the Tier 3 method is not available for all plants, Tier 2 could be used for the remaining plants. If a mix of Tiers is used, it is *good practice* to report the lower Tier as the applied method. If the estimation uses a mix of *c* and *b* Tiers, it is *good practice* to report as method the one giving the highest uncertainty.

To avoid double counting, emissions from the production of hydrogen as a by-product or intermediate product being reported under other sectors, including Ammonia production and Methanol production (IPPU), Petroleum refining (Energy), must be excluded from hydrogen production.

Recovered CO_2 which is used in downstream sectors or sent to permanent storage should be subtracted from hydrogen production, to avoid double counting with downstream sectors.

Biogenic CO_2 emissions should be excluded from the Hydrogen production sector and allocated to a memo item, to avoid double counting with the AFOLU sector.

See Box 3.16 for more details on double counting and gaps.

3.11.2.5 DEVELOPING A CONSISTENT TIME SERIES

Recalculation of CO_2 emissions should be made for all years whenever emission calculation methods are changed (e.g., if the inventory compiler changes from the use of default values to actual values determined at the plant level). If plant-specific data on hydrogen production and consumed feedstock, and data on recovered CO_2 and stored C, are not available for all years in the time series, it will be necessary to consider how current data can be used to recalculate emissions for previous years. It may be possible to apply current factors to data from previous years, provided that the production technology has not changed substantially.

Recalculation is required to ensure that any changes in emissions trends are real and not an artefact of changes in estimation methods. It is *good practice* to recalculate the time series according to the guidance provided in Volume 1, Chapter 5.

3.11.3 Uncertainty assessment

3.11.3.1 EMISSION FACTOR UNCERTAINTIES

It is *good practice* to obtain uncertainty estimates at the same level (i.e. national, regional or plant) as the activity data. In case of plant level data, the uncertainty should be lower than uncertainty values associated with default values. The same applies to country-specific factors.

Feedstock requirement factors (FRFs): Uncertainty in the default FRFs arise from variation between plants in how efficiently the hydrogen is produced. Three factors are decisive to the level of uncertainty: 1) the process efficiency, i.e. how much fuel is combusted for process heat per tonne of produced hydrogen, 2) the chemical composition of the feedstock, i.e. the hydrogen to carbon ratio, and 3) the specific energy content of the feedstock. Feedstock specific factors have lower uncertainty than the general default factor, because the latter contain the variation in process efficiency, chemical composition and specific energy content between different types of feedstock. Plant specific factors have even lower uncertainties. Estimation methods using FRFs (Tier *b* and *a* methods) have higher overall uncertainty than methods not using the fuel requirement factors (Tier *c* methods), *ceteris paribus*, because the Tier *b* and *a* methods include one uncertain element (FRF) that is not included in the Tier *c* methods.

Carbon content factors (CCFs): Uncertainty in the default CCFs is resulting from variation in 1) the chemical composition of the feedstock, i.e. the hydrogen to carbon ratio, and 2) the specific energy content of the feedstock. Uncertainty arise from variation in composition and energy content of a specific material used as feedstock (for example between different types of coal), and from variation in composition and energy content of feedstocks with a heterogeneous composition (for example waste). Feedstock specific factors have lower uncertainty than the general default factor, because the latter contain the variation between different types of feedstock. Plant specific factors have even lower uncertainties.

In the Tier 1a method, if the highest default CCF value among the feedstock types used in the country is used for the entire production, a country-specific uncertainty estimate or alternatively a default *increase* in the remaining uncertainty of 20 percentage points in the downward direction (only) should be used.

3.11.3.2 ACTIVITY DATA UNCERTAINTIES

Where the activity data are obtained at the plant-specific level, uncertainty estimates may be obtained directly from the hydrogen producers. These activity data are likely to be highly accurate (i.e., with uncertainty as low as ±2 percent). This includes uncertainty estimates for feedstock use (Tier *c* methods) or hydrogen production (Tier *b* and *a* methods), as well as CO_2 recovered and stored solid carbon. Data that are obtained from national statistical agencies usually do not include uncertainty estimates. It is *good practice* to consult with national statistical agencies to obtain information on any uncertainty. Where national statistical agencies collect data from the population of hydrogen production facilities, uncertainties in national statistics are not expected to differ from uncertainties established from plant-level consultations. Where uncertainty values are not available from other sources, a default value of ±5 percent can be used for activity data from national statistical agencies.

If plant-specific data are not available for all years in the time series, and current data are used to recalculate emissions for previous years, the uncertainty in emission estimates might increase due to changes in production technology. It is *good practice* to increase the uncertainty values accordingly.

Where uncertainty values are not available from other sources, a default increase of ±20 percent in the uncertainty can be used for previous reference years estimates based on data on current years.

Where estimates are made to split the fossil and biogenic parts of a mixed feedstock in the Tier 1 and 2 methods, a default uncertainty of ±5 percent should be added to the biogenic part if it is based on reported figures, and ±20 percent if it is estimated. The same uncertainty, in absolute amounts, should be added to the fossil part.

3.11.4 Quality Assurance/Quality Control (QA/QC), Reporting and Documentation

3.11.4.1 QUALITY ASSURANCE/QUALITY CONTROL

It is *good practice* to conduct quality control checks as outlined in Volume 1, Chapter 6. More extensive quality control checks and quality assurance procedures are applicable, if higher tier methods are used to determine emissions. Inventory compilers are encouraged to use higher tier QA/QC for *key categories* as identified in Volume 1, Chapter 4.

Comparison of emission factors

Inventory compilers should check if the estimated factors are within the range of default factors, and also ensure that the emission factors are consistent with the values derived from analysis of the process chemistry. For example, the CO_2 generation rate based on natural gas should not be less than 5.46 tonne of CO_2 per tonne of hydrogen produced[7]. If the emission factors are outside of the estimated range of default factors, it is *good practice* to assess and document the plant-specific or country-specific conditions that account for the differences.

Comparison of activity data

It is useful to collect and report activity data comprising both process input data (feedstock consumption) and process output data (hydrogen production), to control the relation between them.

It is *good practice* to cross-check that all emissions from downstream use of recovered CO_2 is accounted for in the corresponding downstream IPPU or other sector(s).

Plant-specific data check

The following plant-specific data are required for adequate auditing of emissions estimates at the Tier 3 level:

- Calculations and estimation method;
- List of assumptions;
- Documentation of any plant-specific measurement method, and measurement results;

QC procedures in use at the site should be directly referenced and included in the QC plan. If the measurement practices were not consistent with QC standards, the inventory compiler should reconsider the use of these data.

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[7] Method: 44.011 tonne CO_2 / 8.064 tonne H = 5.46 tonne of CO_2 per tonne of H_2 produced, based on molar weights of 12.011 (C), 16.00 (O), 1.008 (H) and 100 percent production yield (i.e. no by-products produced, no fuel combustion to produce heat and no feedstock loss in the production process).

3.11.4.2 REPORTING AND DOCUMENTATION

It is *good practice* to document and archive all information required to produce the national emissions inventory estimates as outlined in Volume 1, Section 6.11.

Some examples of specific documentation and reporting that may be relevant to this source category are provided below:

- Description of the method used;
- Number of hydrogen main product production plants;
- Feedstock requirement factors;
- Carbon content factors;
- Feedstock consumption data;
- Production data;
- Production capacity;
- CO_2 recovery data;
- Downstream use and permanent storage of recovered CO_2;
- Stored solid carbon data;
- Any other assumptions.

Ideally, plant operators should supply this information to the inventory compiler for compilation, and also archive the information at the site. Plant operators should also log and archive the measurement frequencies and instrumental calibration records where actual plant measurements are made.

Where such inventory data (e.g. plant- or company-specific production data) may be considered confidential (e.g. where there are only one or two producers in a country), then inventory compilers should refer to guidance presented in Volume 1, Chapter 2 *Approaches to Data Collection*. In these cases, operators and the inventory compiler should seek to determine the level of aggregation at which information can be reported while still protecting confidentiality. Detailed information including instrumentation records should still be archived at the plant level.

It is not practical to include all documentation in the national inventory report. However, the inventory should include summaries of methods used and references to source data such that the reported emissions estimates are transparent and steps in their calculation may be retraced.

ANNEX 3A.1 DEFAULT EMISSION FACTORS FOR SECTION 3.10.2 EMISSIONS FROM PRODUCTION OF FLUORINATED COMPOUNDS (OTHER THAN HFC-23 EMISSIONS FROM HCFC-22 PRODUCTION)

This annex provides background information for the Tier 1 default emission factors for fluorinated greenhouse gases (GHG) from fluorochemical production, that are provided in section 3.10.2 in the *2019 Refinement* to the *2006 IPCC Guidelines*. The first section discusses the default emission factors for SF_6 and NF_3 production based on literature search, and the second section discusses the default emission factor estimated from the data reported to the U.S. Greenhouse Gas Reporting Program.

EXECUTIVE SUMMARY

The Tier 1 default emission factor for production of fluorinated gases other than SF_6 and NF_3 was developed based on emissions and throughput (production and transformation) information reported to the U.S. Greenhouse Gas Reporting Program (GHGRP). The factor is intended to represent uncontrolled emissions. Under the GHGRP, fluorinated GHG emissions are reported annually on a facility basis and include facilities with and without abatement. Depending on the year, 14 to 16 fluorochemical production facilities have reported under the Program. Facilities that abate their emissions report their level of abatement for each process as a range. To develop emission factors on an uncontrolled basis, the pre-abatement emissions of each facility were estimated using the arithmetic averages of the abatement ranges reported by that facility for its processes. Then, for each facility, this estimate was divided by the total quantity of fluorinated gases produced or transformed by that facility to obtain an uncontrolled emission factor for that facility and year. This was done for all six years for which the US EPA had data at the time the factor was developed. For each facility, the emission factors for each year were then averaged over the six years of reporting, and the resulting facility averages were averaged to obtain the default factor. Because the reporting U.S. facilities use multiple manufacturing methods to produce a wide array of fluorochemicals, averaging the facility-specific emission factors is expected to provide a default emission factor that is applicable where the manufacturing method is unknown, as is often the case in a Tier 1 calculation.

The uncertainty of the default emission factor was assessed using several methods, including sensitivity analyses, Monte Carlo analysis, and statistical analyses. As discussed further below in section 3A.1.5, these analyses showed that the selected factor was robust despite uncertainties in the reported data, such as the reporting of destruction efficiencies as a range rather than a single value. However, the analyses also indicated that the uncertainty in the emission factor for any single facility is quite large, and is dictated by the fact that true uncontrolled emission rates naturally vary from facility to facility depending on the fluorochemicals produced and the type of manufacturing method used to produce them.

3A.1.1 BACKGROUND INFORMATION FOR SECTION 3.10.2 TIER 1 DEFAULT EMISSION FACTORS – FROM THE LITERATURE

The literature shows a broad range of emission factors for different gases and even for the same gas when it is produced for different applications. For SF_6 produced in Japan, a factor of 0.08 kg emitted/kg produced was found for facilities whose customers require highly purified SF_6 gas (e.g., semiconductor manufacturing). The emission factor is relatively large because of handling losses during disposal of residual gas (i.e., the 'heel' that is not used or recycled) in returned cylinders (Suizu, 1999). An SF_6 emission factor has been reported as 0.03 kg emitted/kg of sales (O'Connell, 2002).

U.S. and Japanese NF_3 manufacturers have reported an emission factor for NF_3 emissions of 0.02 in 2009, with a goal of eventually achieving an emission factor of 0.005 kg emitted/kg produced (it is not known whether the 0.005 factor is based on pre-abatement emissions or controlled, post-abatement emissions) (Fthenakis, 2010). CF_4 and N_2O are generated as a by-product during NF_3 manufacture, and N_2O and CF_4 can be formed at rates of 0.03 kg emitted/kg produced and less than 0.01 kg emitted/kg produced, respectively, relative to the mass of NF_3 formed during electrolysis (these emission factors are on an uncontrolled, pre-abatement basis) (Tasaka, 2004; 2007). Some process-specific emission factor data are available from commercially available life cycle assessment software; these EFs may be acceptable should sufficient documentation of their units, source data, and calculation exist.

In another reference focused on SF_6 produced in Germany, an emission factor of 0.002 kg emitted/kg of the total quantity of SF_6 produced was found for facilities whose customers do not require highly purified SF_6 gas (e.g., electrical equipment, insulated windows) (Preisegger, 1999). Unfortunately, it is not known whether the 0.002

kg emitted/kg produced factor is based on pre-abatement emissions or controlled, post-abatement emissions, and therefore it should not be used for Tier 1 estimates. The authors note the value here for informational purposes and to acknowledge that the data were reviewed for the Tier 1 methodology.

3A.1.2 BACKGROUND INFORMATION FOR SECTION 3.10.2 TIER 1 DEFAULT EMISSION FACTORS – ALL OTHER FLUORINATED GHG

3A.1.2.1 Source of Data

The U.S. GHGRP[8] requires certain facilities that emit greenhouse gases (GHGs) and certain suppliers of fossil fuels and industrial GHGs to report their emissions or supplies (along with other relevant data) annually to the US Environmental Protection Agency (EPA). In general, reporting requirements apply to facilities or suppliers that meet or exceed thresholds that are equivalent to emissions of 25,000 metric tonne of CO_2 equivalent (CO_2eq.) per year. Facilities and reporters collect data for the calendar year and report those data to EPA electronically in the following year by March 31.[9] The US EPA verifies[10] the data and then publishes it. The GHGs covered include carbon dioxide (CO_2), methane (CH_4), nitrous oxide (N_2O), hydrofluorocarbons (HFCs), perfluorocarbons (PFCs), sulphur hexafluoride (SF_6), and other fluorinated gases (e.g., nitrogen trifluoride, hydrofluoroethers [HFEs], perfluorinated amines, etc.).

The default emission factor for fluorochemical production is based on data reported under two sections of the GHGRP regulation—subpart L, Fluorinated Gas Production, and subpart OO, Suppliers of Industrial Greenhouse Gases—for reporting years (RY)[11] 2011 to 2016. Under subpart L, facilities that produce a fluorinated gas (other than HCFC-22[12]) must report their fluorinated GHG emissions from the production and transformation of fluorinated gases, from venting of residual fluorinated GHGs from containers, and from destruction of previously produced fluorinated GHGs. The emissions reported from production and transformation include both emissions from process vents and emissions from equipment leaks. Under subpart OO, fluorinated GHG suppliers (including fluorinated GHG producers) must report the quantities of each fluorinated GHG that they produce, transform, destroy, import, or export.

3A.1.2.2 Data Used in Development of the Fluorinated GHG Emissions Factor

The emission factor was developed from: (1) the emissions from production and transformation processes and emissions from venting of residual fluorinated GHGs from containers, and (2) the quantities of fluorinated GHGs produced and transformed. Facilities reporting emissions under subpart L provide information on emissions from production and transformation processes at two levels of aggregation and in two metrics:

- For the facility as a whole, emissions are provided by specific fluorinated GHG compound in metric tonne where the facility makes more than one product and where the emissions of that compound equal or exceed 1,000 metric tonne CO_2eq. across all processes. Where total emissions of a compound across all processes are less than 1,000 metric tonne CO_2eq., emissions are reported by fluorinated GHG group[13] in metric tonne CO_2eq. Where the facility makes only one product, emissions are reported by compound when that compound is the same as the product; otherwise they are reported by fluorinated GHG group in metric tonne CO_2eq.
- For each production and transformation process at the facility, emissions are reported by process and fluorinated GHG group in metric tonne CO_2eq.

The global warming potentials (GWPs) used to calculate CO_2-equivalent emissions are drawn from the IPCC Fourth Assessment Report (AR4), IPCC Fifth Assessment Report (AR5), or then a default GWP is used. For

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[8] The GHGRP regulation can be found in the U.S. Code of Federal Regulations (CFR) at Title 40, Part 98. For background information on and data from the GHGRP, please see <https://www.epa.gov/ghgreporting>

[9] Mandatory Reporting of Greenhouse Gases. Final rule. (74 FR 56260). October 30, 2009.

[10] For information on how EPA verifies data submitted under the GHGRP, please see <https://www.epa.gov/sites/production/files/2015-07/documents/ghgrp_verification_factsheet.pdf>.

[11] The term “reporting year (RY)” refers to the year in which the emissions occurred.

[12] Facilities that produce HCFC-22 are required to report their emissions under a separate part of the GHGRP, Subpart O. The emission factor being developed here is intended to apply to production of fluorochemicals other than HCFC-22 (which is covered in section 3.10.1 of the *F*), and therefore emissions from HCFC-22 production are not discussed further here.

[13] There are twelve fluorinated GHG groups, each of which encompasses a set of GHGs with roughly similar atmospheric behaviour, including similar GWPs and atmospheric lifetimes. These include, e.g., fully fluorinated GHGs such as PFCs and SF_6, HFCs with two or fewer hydrogen-carbon bonds, HFCs with more than two carbon-hydrogen bonds, unsaturated HFCs and PFCs, etc. (See Table A3.1.3 for a full list.) Compounds that do not have GWPs in either the Fourth Assessment Report (AR4) or AR5 are assigned a default GWP that is generally based on the average GWP for the fluorinated GHG group of which the compound is a member.

most fluorinated GHG groups, the default GWP is the average of the GWPs of all the fluorinated GHGs in that group that have GWP values in AR4 or AR5.[14] Where we use emissions reported in CO_2eq. in our calculations, we back-calculate the emissions in metric tonne using the same set of GWPs used to calculate the CO_2eq. emissions.

For the processes, facilities also report the range into which the destruction efficiency (DE) of each process falls. (The DE is based on the extent to which emissions from process vents are controlled. Emissions from equipment leaks are not included in the DE calculation.) Table 3A.1.1 provides the DE ranges available for facilities to report and the DE assumptions for each.

TABLE 3A.1.1 (NEW)
DESTRUCTION EFFICIENCY RANGE VALUES USED TO ESTIMATE PRE-ABATEMENT EMISSIONS FOR PRODUCTION AND TRANSFORMATION PROCESSES

DE ranges	Lower Bound	Upper Bound	Arithmetic Mean of Bounds	Geometric Mean of Bounds
>=0% to <75%	0.0	0.75	0.375	0.500
>=75% to <95%	0.75	0.95	0.85	0.888
>=95% to <99%	0.95	0.99	0.97	0.978
>=99%	0.99	0.9999	0.995	0.999

Facilities reporting emissions of residual fluorinated GHGs from container venting report emissions in metric tonne of each fluorinated GHG.

The activity data for the emission factor was compiled from reporting of the quantities of fluorinated GHGs produced and transformed that were reported under subpart OO.

A3.1.2.3 Calculation of Emissions from Production and Transformation Processes

a. Actual Emissions by Specific Fluorinated GHG for Production and Transformation Processes

Actual emissions of specific fluorinated GHGs reported under subpart L for production and transformation processes are provided in Table 3A.1.2. Table 3A.1.2 provides actual emissions by specific fluorinated GHG for production and transformation processes in metric tonne, and also provides actual GWP-weighted emissions by specific fluorinated GHG for production and transformation processes in metric tonne CO_2eq. Actual emissions are those emissions that actually occur to the atmosphere and reflect the level of control for the process. These totals include only the portion of production and transformation process emissions that are reported by specific fluorinated GHG (approximately 98 percent of production and transformation emissions in metric tonne CO_2eq.).[15]

b. Actual Emissions by Fluorinated GHG Group

Actual emissions of fluorinated GHGs reported under subpart L are provided by fluorinated GHG group for each production and transformation process. Table 3A.1.3 provides actual fluorinated GHG emissions in metric tonne CO_2eq. by fluorinated GHG group. The group totals include all emissions from production and transformation processes.

c. Estimated Emissions Prior to Control by Fluorinated GHG Group

Uncontrolled emissions (i.e., pre-abatement emissions) for production and transformation processes were estimated based on the destruction efficiency (DE) range provided by facilities when they reported on each process, along with the actual fluorinated GHG emissions reported in metric tonne CO_2eq. Because facilities provide the range in which the DE falls rather than the exact DE, an assumption of the true DE must be made.

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[14] For fluorinated GHG groups that have average GWPs below one, including unsaturated HFCs and PFCs, fluorotelomer alcohols, and compounds with carbon-iodine bonds, a default value of one is used, but as discussed further below, these compounds are excluded from this analysis.

[15] The tables in this discussion and subsequent estimated pre-abatement emission discussions exclude compounds with GWPs near or below 1 (i.e., unsaturated PFCs, HFCs, etc.; fluorotelomer alcohols; and fluorinated GHGs with carbon-iodide bonds) because these compounds account for only 0.01 percent of the GWP-weighted emissions reported under subpart L and, as discussed further in section A3.1.5, including them introduces large uncertainties into the emission factor expressed in units of metric tonne.

TABLE 3A.1.2 (NEW)
ACTUAL EMISSIONS FROM PRODUCTION AND TRANSFORMATION PROCESS REPORTED BY SPECIFIC FLUORINATED GHG UNDER SUBPART L OF THE GHGRP (CONSIDERING CONTROLS) (APPROXIMATELY 98 PERCENT OF P/T PROCESS EMISSIONS IN METRIC TONNE CO_2 EQUIVALENT), METRIC TONNE AND METRIC TONNE CO_2 EQUIVALENT[A]

Fluorinated GHG Name	2011	2012	2013	2014	2015	2016	Sum Total, tonne	% tonne	Cumulative %	2011	2012	2013	2014	2015	2016	Sum Total, tonne CO_2eq.	% tonne CO_2eq.	Cumulative %
HFC-134a	266	222	208	203	227	147	1,273	20%	20%	380,008	317,799	297,074	290,333	324,151	210,574	1,819,938	5.0%	5.0%
HFC-23	191	214	198	112	81	53	849	13%	33%	2,829,581	3,166,284	2,934,831	1,661,087	1,191,554	778,851	12,562,188	34.4%	39.4%
HFC-125	152	151	156	151	136	63	808	12%	45%	533,042	528,308	545,053	527,997	475,389	219,482	2,829,271	7.7%	47.1%
HFC-32	155	165	152	116	130	91	808	12%	58%	104,652	111,119	102,620	78,408	87,501	61,176	545,475	1.5%	48.6%
HFC-143a	136	127	128	100	93	102	685	11%	68%	607,421	566,428	570,420	446,846	413,610	456,470	3,061,194	8.4%	57.0%
PFC-14 (Perfluoromethane)	60	77	58	47	46	54	342	5%	73%	445,137	568,391	428,165	346,613	336,266	402,576	2,527,148	6.9%	63.9%
HFC-245fa	48	49	49	50	41	41	278	4%	78%	49,595	49,965	50,048	51,510	42,477	42,371	285,966	0.8%	64.7%
Perfluorocyclobutane	53	35	26	29	28	52	223	3%	81%	546,574	362,868	268,346	296,849	290,191	535,633	2,300,460	6.3%	71.0%
HFC-227ea	26	25	35	24	25	23	158	2%	84%	84,275	81,365	112,449	76,572	81,943	72,729	509,332	1.4%	72.4%
PFC-116 (Perfluoroethane)	21	20	40	17	23	2	123	2%	86%	250,244	246,574	485,921	207,274	284,305	21,572	1,495,890	4.1%	76.4%
Nitrogen trifluoride	31	28	20	16	15	13	122	2%	87%	531,201	482,591	336,165	272,076	261,263	218,992	2,102,289	5.8%	82.2%
Octafluorotetrahydrofuran	19	25	40	23	6	5	117	2%	89%	188,440	253,010	395,575	232,025	56,124	48,225	1,173,399	3.2%	85.4%
Hexafluoropropylene oxide	11	17	19	20	23	18	109	2%	91%	114,620	172,341	190,459	197,199	233,900	179,593	1,088,112	3.0%	88.4%
PFC-218 (Perfluoropropane)	12	7	48	16	3	3	89	1%	92%	106,887	62,557	424,737	143,241	28,298	23,976	789,696	2.2%	90.6%
Pentafluoro(trifluoromethyl)-cyclopropane	10	8	10	11	19	15	75	1%	93%	102,885	82,428	103,221	112,075	192,068	152,615	745,292	2.0%	92.6%
HFE-449sl, (HFE-7100) Isomer blend	11	11	12	9	9	11	62	1%	94%	3,191	3,264	3,578	2,734	2,598	3,195	18,559	0.1%	92.6%
PFC-5-1-14 (Perfluorohexane, FC 72)	12	8	8	10	13	6	57	1%	95%	109,192	76,500	73,980	95,154	118,276	56,068	529,169	1.4%	94.1%
HFC-152a	9	9	12	0	0	21	51	1%	96%	1,089	1,152	1,491	0	0	2,633	6,366	0.0%	94.1%
Trifluoromethyl sulphur pentafluoride	8	9	19	5	3	2	45	1%	97%	136,465	166,270	332,625	92,038	47,636	29,748	804,783	2.2%	96.3%
1,1,1,2,2,3,3-Heptafluoro-3-(1,2,2,2-tetrafluoroethoxy)-propane	0	0	4	7	6	15	33	1%	97%	3,019	3,162	24,892	42,564	41,909	97,311	212,857	0.6%	96.9%

Table 3A.1.2 (New) (Continued)
Actual emissions from production and transformation process reported by specific fluorinated GHG under Subpart L of the GHGRP (considering controls) (approximately 98 percent of P/T process emissions in metric tonne CO_2 equivalent), metric tonne and metric tonne CO_2 equivalent

Fluorinated GHG Name	2011	2012	2013	2014	2015	2016	Sum Total, tonne	% tonne	Cumulative %	2011	2012	2013	2014	2015	2016	Sum Total, tonne CO_2eq.	% tonne CO_2eq.	Cumulative %
2H-perfluoro(5-methyl-3,6-dioxanonane)	4	5	3	2	2	6	21	0%	98%	7,776	9,072	6,125	3,462	4,604	11,015	42,053	0.1%	97.0%
Trifluoromethanesulfonyl fluoride	3	4	6	4	2	1	20	0%	98%	6,552	8,400	12,221	7,502	3,111	2,799	40,584	0.1%	97.1%
HFC-236fa	2	3	5	3	2	2	17	0%	98%	22,152	33,285	47,912	28,497	18,093	14,821	164,760	0.5%	97.6%
PFC-3-1-10 (Perfluorobutane)	2	2	6	3	1	2	15	0%	98%	17,853	13,349	54,566	23,017	9,143	18,817	136,746	0.4%	97.9%
Perfluorodiethyl ether	2	3	2	1	2	2	11	0%	99%	16,779	29,448	21,421	13,619	16,460	16,236	113,963	0.3%	98.3%
Perfluorobutanesulfonyl fluoride	1	1	1	1	1	5	10	0%	99%	2,431	1,674	2,091	1,840	2,658	10,155	20,850	0.1%	98.3%
Sulfur hexafluoride	1	1	3	3	1	0	10	0%	99%	28,991	25,709	73,509	66,975	23,181	5,910	224,276	0.6%	98.9%
Pentafluoro(trifluoromethoxy)-ethane	2	1	3	1	1	0	8	0%	99%	19,298	10,784	29,517	10,139	5,747	4,844	80,329	0.2%	99.1%
Hexafluorooxetane	1	1	4	1	1	1	8	0%	99%	13,921	9,418	35,195	6,581	7,064	6,035	78,214	0.2%	99.4%
PFC-4-1-12 (Perfluoropentane)	2	1	1	1	2	1	8	0%	99%	18,958	8,201	9,053	5,933	15,605	13,627	71,377	0.2%	99.6%
Carbonyl fluoride	1	1	1	1	1	1	6	0%	99%	2,977	1,673	1,340	1,803	1,584	2,492	11,869	0.0%	99.6%
Trifluoroacetyl fluoride	1	1	1	1	1	1	5	0%	99%	2,493	1,654	1,339	1,638	1,651	1,890	10,664	0.0%	99.6%
HFC-43-10mee	1	1	1	1	0	1	5	0%	100%	1,657	1,504	1,673	1,163	0	1,529	7,526	0.0%	99.6%
Perfluoropropionyl fluoride	1	1	1	1	1	0	4	0%	100%	1,928	1,661	2,261	1,077	1,619	0	8,546	0.0%	99.7%
Perfluoro-2-(2-fluorosulfonylethoxy) propyl vinyl ether	0	0	0	0	1	3	4	0%	100%	0	0	0	0	2,167	5,654	7,821	0.0%	99.7%
2,2,3,3,4-Pentafluro-4-(trifluoromethyl)-oxetane	0	1	2	0	0	0	3	0%	100%	3,111	8,787	16,370	3,665	1,530	1,009	34,472	0.1%	99.8%
HFC-365mfc	0	0	3	0	0	0	3	0%	100%	0	0	2,620	0	0	0	2,620	0.0%	99.8%
PFC-6-1-12	1	1	0	0	0	0	3	0%	100%	8,867	10,099	1,078	1,110	2,219	0	23,373	0.1%	99.8%
Isobutyryl fluoride	2	0	0	0	0	0	2	0%	100%	4,668	0	0	0	0	0	4,668	0.0%	99.9%

TABLE 3A.1.2 (NEW) (CONTINUED)
ACTUAL EMISSIONS FROM PRODUCTION AND TRANSFORMATION PROCESS REPORTED BY SPECIFIC FLUORINATED GHG UNDER SUBPART L OF THE GHGRP (CONSIDERING CONTROLS) (APPROXIMATELY 98 PERCENT OF P/T PROCESS EMISSIONS IN METRIC TONNE CO_2 EQUIVALENT), METRIC TONNE AND METRIC TONNE CO_2 EQUIVALENT

Fluorinated GHG Name	2011	2012	2013	2014	2015	2016	Sum Total, tonne	% tonne	Cumulative %	2011	2012	2013	2014	2015	2016	Sum Total, tonne CO_2eq.	% tonne CO_2eq.	Cumulative %
1,1,1,3,3,5,5,7,7,9,9,11,11-tridecafluoro-2,4,6,8,10-pentaoxadodecan-12-oyl fluoride	0	0	0	0	1	0	1	0%	100%	0	0	0	0	2,993	0	2,993	0.0%	99.9%
HFC-227ca	0	0	1	0	0	0	1	0%	100%	0	1,120	2,727	0	0	0	3,846	0.0%	99.9%
2,3,3,3-Tetrafluoro-2-(trifluoromethoxy)propionyl fluoride	1	1	0	0	0	0	1	0%	100%	1,141	1,176	0	0	0	0	2,317	0.0%	99.9%
Heptafluoropropyl trifluoromethyl ether	0	0	0	0	0	0	1	0%	100%	1,299	1,004	3,103	0	1,143	2,086	8,635	0.0%	99.9%
2-Butene, 2-chloro-1,1,1,3,4,4,4-heptafluoro	1	0	0	0	0	0	1	0%	100%	1,380	0	0	0	0	0	1,380	0.0%	99.9%
Trifluoroacetic acid	0	0	1	0	0	0	1	0%	100%	0	0	1,378	0	0	0	1,378	0.0%	99.9%
1H-perfluorooctane	0	0	0	0	0	1	1	0%	100%	0	0	0	0	0	2,404	2,404	0.0%	99.9%
Unknown FC	0	0	0	0	0	0	1	0%	100%	0	0	0	0	2,267	3,888	6,155	0.0%	99.9%
[[Difluoro(trifluoromethoxy)methoxy]difluoromethoxy]difluoro-acetyl fluoride	0	0	0	0	0	1	1	0%	100%	0	0	0	0	0	1,190	1,190	0.0%	99.9%
Propanenitrile, 2,3,3,3-tetrafluoro-2-(trifluoromethyl)-	0	0	0	0	0	1	1	0%	100%	0	0	0	0	0	1,091	1,091	0.0%	99.9%
Unknown Sulfonated FC	0	0	0	0	0	0	1	0%	100%	0	0	3,143	1,036	0	1,238	5,417	0.0%	100.0%
Perfluoro compounds, C5-18	0	0	0	0	0	0	0	0%	100%	0	0	39	837	0	4,034	4,910	0.0%	100.0%
C5F13N	0	0	0	0	0	0	0	0%	100%	1,545	0	0	0	1,055	0	2,600	0.0%	100.0%
Perfluorotributyl amine	0	0	0	0	0	0	0	0%	100%	1,179	1,058	0	0	0	0	2,237	0.0%	100.0%
C6F15N	0	0	0	0	0	0	0	0%	100%	2,021	0	0	0	0	0	2,021	0.0%	100.0%
C7F16O	0	0	0	0	0	0	0	0%	100%	0	0	1,474	0	0	0	1,474	0.0%	100.0%
C6F12	0	0	0	0	0	0	0	0%	100%	0	0	0	0	1,015	0	1,015	0.0%	100.0%
Perfluorobutyliodide	-	-	-	-	-	-	-	0%	100%	-	-	-	-	-	-	-	-	100.0%
HFC-1132a; VF2	-	-	-	-	-	-	-	0%	100%	-	-	-	-	-	-	-	-	100.0%
HFC-1141; VF	-	-	-	-	-	-	-	0%	100%	-	-	-	-	-	-	-	-	100.0%
1,1,1,3,3,3-Hexafluropropane	-	-	-	-	-	-	-	0%	100%	-	-	-	-	-	-	-	-	100.0%

Table 3A.1.2 (New) (Continued)
Actual emissions from production and transformation process reported by specific fluorinated GHG under Subpart L of the GHGRP (considering controls) (approximately 98 percent of P/T process emissions in metric tonne CO_2 equivalent), metric tonne and metric tonne CO_2 equivalent

Fluorinated GHG Name	2011	2012	2013	2014	2015	2016	Sum Total, tonne	% tonne	Cumulative %	2011	2012	2013	2014	2015	2016	Sum Total, tonne CO_2eq.	% tonne CO_2eq.	Cumulative %
1,2-Oxathiane, 3,3,4,4,5,5,6,6-octafluoro-, 2,2-dioxide	-	-	-	-	-	-	-	0%	100%	-	-	-	-	-	-	-	-	100.0%
2,2,3,3,4,4,-hexafluoro-4-(fluorosufonyl)-butanoyl fluoride	-	-	-	-	-	-	-	0%	100%	-	-	-	-	-	-	-	-	100.0%
2,3,3,3-Tetrafluoro-2-(heptafluoropropoxy)propanoyl fluoride	-	-	-	-	-	-	-	0%	100%	-	-	-	-	-	-	-	-	100.0%
Heptafluoropropyl trifluorovinyl ether	-	-	-	-	-	-	-	0%	100%	-	-	-	-	-	-	-	-	100.0%
Hexafluoroacetone	-	-	-	-	-	-	-	0%	100%	-	-	-	-	-	-	-	-	100.0%
HFC-236ea	-	-	-	-	-	-	-	0%	100%	-	-	-	-	-	-	-	-	100.0%
Methyl perfluoro(5-methyl-4,7-dioxanon-8-enoate)	-	-	-	-	-	-	-	0%	100%	-	-	-	-	-	-	-	-	100.0%
Oxetane, 2,2,3,4,4-Pentafluro-3-(trifluoromethyl)-	-	-	-	-	-	-	-	0%	100%	-	-	-	-	-	-	-	-	100.0%
Pentafluoroethyl trifluorovinyl ether	-	-	-	-	-	-	-	0%	100%	-	-	-	-	-	-	-	-	100.0%
Perfluoroisobutyric acid fluoride	-	-	-	-	-	-	-	0%	100%	-	-	-	-	-	-	-	-	100.0%
PFC-1114; TFE	-	-	-	-	-	-	-	0%	100%	-	-	-	-	-	-	-	-	100.0%
PFC-1216; Dyneon HFP	-	-	-	-	-	-	-	0%	100%	-	-	-	-	-	-	-	-	100.0%
PMVE; HFE-216	-	-	-	-	-	-	-	0%	100%	-	-	-	-	-	-	-	-	100.0%
Propanoyl fluoride, 2,2,3,3-tetrafluoro-	-	-	-	-	-	-	-	0%	100%	-	-	-	-	-	-	-	-	100.0%
1,2-Oxathiane, 3,3,4,4,5,5,6,6-octafluoro-, 2,2-dioxide	-	-	-	-	-	-	-	0%	100%	-	-	-	-	-	-	-	-	100.0%
2,2,3,3,4,4,-hexafluoro-4-(fluorosufonyl)-butanoyl fluoride	-	-	-	-	-	-	-	0%	100%	-	-	-	-	-	-	-	-	100.0%
TOTAL	1,263	1,237	1,285	988	946	765	6,484			7,316,491	7,481,451	8,011,806	5,352,488	4,634,366	3,746,556	36,543,158		

[a] US EPA, 2017. Data extracted from US EPA Facility Level Information on Greenhouse Gases Tool (FLIGHT). Based on data reported to EPA by August 05, 2017 (freeze date). https://ghgdata.epa.gov/ghgp/main.do#

TABLE 3A.1.3 (NEW)
ACTUAL FLUORINATED GHG EMISSIONS FROM PRODUCTION AND TRANSFORMATION PROCESSES FROM SUBPART L OF THE GHGRP (CONSIDERING CONTROLS), BY GROUP (METRIC TONNE CO_2 EQUIVALENT) [A]

Fluorinated GHG Group	**2011**	**2012**	**2013**	**2014**	**2015**	**2016**
Fully fluorinated GHGs	2,679,675	2,609,942	3,313,760	2,149,381	1,942,407	1,756,714
Saturated hydrofluorocarbons (HFCs) with 2 or fewer carbon-hydrogen bonds	4,068,950	4,350,171	4,065,235	2,684,590	2,198,462	1,380,406
Saturated HFCs with 3 or more carbon-hydrogen bonds	677,653	630,075	634,337	507,953	497,508	502,570
Saturated hydrofluoroethers (HFEs) and hydrochlorofluoroethers (HCFEs) with 1 carbon-hydrogen bond	3,324	3,358	25,048	42,617	42,781	97,454
Saturated HFEs and HCFEs with 2 carbon-hydrogen bonds	70	3	4	2	48	67
Saturated HFEs and HCFEs with 3 or more carbon-hydrogen bonds	3,741	4,130	4,743	3,777	4,124	5,289
Fluorinated formates	-	-	-	-	-	0
Fluorinated acetates, carbonofluoridates, and fluorinated alcohols other than fluorotelomer alcohols	62	17	93	243	120	126
Unsaturated perfluorocarbons (PFCs), unsaturated HFCs, unsaturated hydrochlorofluorocarbons (HCFCs), unsaturated halogenated ethers, unsaturated halogenated esters, fluorinated aldehydes, and fluorinated ketones	Excluded from analysis	Excluded from analysis	Excluded from analysis	Excluded from analysis	Excluded from analysis	Excluded from analysis
Fluorotelomer alcohols	Excluded from analysis	Excluded from analysis	Excluded from analysis	Excluded from analysis	Excluded from analysis	Excluded from analysis
Fluorinated GHGs with carbon-iodine bond(s)	Excluded from analysis	Excluded from analysis	Excluded from analysis	Excluded from analysis	Excluded from analysis	Excluded from analysis
Other fluorinated GHGs	40,242	34,485	39,559	25,826	27,114	69,038
TOTAL	**7,473,716**	**7,632,181**	**8,082,779**	**5,414,389**	**4,712,564**	**3,811,664**

[a] Ibid EPA 2017.

We reviewed four DE assumptions, along with the uncontrolled emissions implied by these assumptions, to ensure that the default emission factor was as robust and accurate as possible.[16] These included:

1. A **lower-bound assumption** that assumed that the DE for each process was always equal to the lower bound of the DE range reported for that process. This results in an absolute lower-bound estimate of uncontrolled emissions. Uncontrolled emissions from any facility cannot fall below the level implied by this assumption.
2. An **upper-bound assumption** that assumed that the DE for each process was always equal to the upper bound of the DE range reported for that process. This results in an absolute upper-bound estimate of uncontrolled emissions.[17] Uncontrolled emissions from any facility cannot fall above the level implied by this assumption.
3. An **arithmetic mean assumption** that assumed that the DE for each process was equal to the straight average of the upper and lower bound of the DE range reported for that process. This is expected to be an unbiased estimator of uncontrolled emissions if a DE is equally likely to fall anywhere within the range and uncontrolled emissions are also equally likely to fall anywhere within the range (that is, uncontrolled emissions across processes and facilities are not expected to be higher at one end of the range than the other).
4. A **geometric mean assumption** that assumed that the DE for each process was equal to 1 minus the geometric mean of the fractions emitted at the DE range bounds reported for that process. (In Excel using MS Excel functions, this is summarized by the formula (1-GEOMEAN((1-LB),(1-UB)). This is expected to be an unbiased estimator of uncontrolled emissions if a DE is equally likely to fall anywhere within the range and uncontrolled emissions, across processes and facilities, grow exponentially as the DE increases.

The emissions prior to control for production and transformation processes are calculated using Equation 3A.1.1.

EQUATION 3A.1.1 (NEW)
EMISSIONS PRIOR TO CONTROL FOR PRODUCTION AND TRANSFORMATION PROCESSES

$$Emissions\ Prior\ to\ Control\ =\ \left[\left(Post-Control\ emissions\ from\ process\ vents\right)\ /\ \left(1-DE\right)\right]$$
$$+\ Emissions\ from\ equipment\ leaks$$

Table 3A.1.4 provides the estimated pre-abatement emissions by fluorinated GHG group (in metric tonne CO_2eq.) when each DE assumption is used to estimate pre-abatement emissions.

d. Selection of Arithmetic Mean as Basis for Estimates.

As the basis for our best estimates of uncontrolled emissions, we considered both the arithmetic and geometric means of the DE ranges. Choosing the appropriate DE assumption is based on the distribution of the emissions within each DE range. If the uncontrolled emissions are increasing exponentially across the range, then application of the geometric mean is more appropriate. If the uncontrolled emissions are constant across the range, then application of the arithmetic mean is more appropriate. Exponentially rising uncontrolled emissions would be consistent with a control strategy that selectively targeted the streams with the highest GWP-weighted emissions. It is clear that facilities tend to prioritize the control of high GWP streams and that this is often the first consideration in determining whether a stream will be controlled. In addition to high GWP, however, facilities also include other considerations in their decisions regarding which streams to send to a destruction device. Other considerations may include technical considerations, regulatory requirements, and safety concerns. Technical considerations include things such as the distance from the process to the destruction device for routing a vent to a control device, or the need to drop down the stream pressure prior to venting to a control device. Some facilities will have the technical expertise to overcome these issues while others may not. Another consideration is regulatory requirements or market forces that may affect whether a stream is controlled. In

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[16] As discussed in section A3.1.5 below, we also performed a Monte Carlo analysis to assess the uncertainty of the emission factor estimate, including the uncertainty of the exact DE as well as other uncertainties.

[17] This is unconditionally true for the first three DE ranges, but for the last one (>99 percent), we must choose a realistic upper bound because using a value of 100 percent would result in infinite pre-abatement emissions. We chose 99.99 percent, but we could have chosen 99.9 or 99.999 percent instead, with a factor of 10 difference either way for the pre-abatement emissions in this DE range. We also used the 99.99 percent upper bound to calculate the arithmetic and geometric means for the highest DE range.

addition, safety is a consideration. For example, there may be instances where the destruction device is down and not operating, and for safety reasons a process that is mid-process may be vented directly to the atmosphere.

Table 3A.1.4 provides the controlled emissions (actual) in metric CO_2eq., as well as the uncontrolled emissions in metric tonne CO_2eq. estimated using the lower bound of the DE range, the arithmetic mean of the DE range, the geometric mean of the DE range, and the upper bound of the DE range. These emissions include the full set of emissions from production and transformation processes. Note that the lower-bound uncontrolled emissions are approximately four times as large as the controlled emissions (though this varies by year). The estimates of uncontrolled emissions under the various DE assumptions span a factor of almost 30: the arithmetic-mean uncontrolled emissions are approximately twice as large as the lower-bound uncontrolled emissions, the geometric-mean uncontrolled emissions are approximately two and a half times as large as the arithmetic-mean uncontrolled emissions, and the upper-bound uncontrolled emissions are approximately seven times as large as the geometric-mean uncontrolled emissions.

TABLE 3A.1.4 (NEW)
ESTIMATED PRE-ABATEMENT FLUORINATED GHG EMISSIONS FROM PRODUCTION AND TRANSFORMATION PROCESSES FROM SUBPART L OF THE GHGRP, ALL DE ASSUMPTIONS (METRIC TONNE CO_2 EQUIVALENT)

DE Assumption	2011	2012	2013	2014	2015	2016	Sum Total, tonne CO_2eq.
Actual emissions	7,473,716	7,632,181	8,082,779	5,414,389	4,712,564	3,811,664	37,127,293
Lower bound DE emissions, pre-abatement	33,126,816	26,348,042	22,970,419	23,678,050	21,459,616	27,852,452	155,435,395
Arithmetic mean DE emissions, pre-abatement	57,275,451	43,684,030	37,104,181	38,859,484	35,409,856	49,860,047	262,193,049
Geometric mean DE emissions, pre-abatement	162,302,698	89,923,131	60,355,569	73,690,456	70,568,769	167,408,713	624,249,337
Upper bound DE emissions, pre-abatement	1,275,608,396	541,882,779	256,555,587	400,139,115	407,755,113	1,441,071,577	4,323,012,567

One author compiled data on DEs achieved for one fluorochemical production process over several years, and these data showed a geometric distribution. However, there was no way to be certain that the distribution for this single process applied to the hundreds of other processes whose emissions are reported under subpart L. Thus, we selected the arithmetic mean, which assumes that uncontrolled emissions are flat as the DE increases, as the basis for our estimates of uncontrolled emissions. For this reason, the detailed analysis below focuses on the arithmetic mean scenario, but summary information is provided for the other scenarios to show the sensitivity of uncontrolled emissions to different DE assumptions. Table 3A.1.5 provides the uncontrolled emissions by fluorinated GHG group (in metric tonne CO_2eq.) estimated using the arithmetic mean of the DE range. The estimates in Table 3A.1.5 are used in section 3.1.4 to develop the profile of specific fluorinated GHGs emitted in a pre-abatement scenario.

TABLE 3A.1.5 (NEW)
ESTIMATED PRE-ABATEMENT FLUORINATED GHG EMISSIONS FROM PRODUCTION AND TRANSFORMATION PROCESSES FROM SUBPART L OF THE GHRP (USING ARITHMETIC MEAN OF DE RANGE), BY FLUORINATED GHG GROUP (METRIC TONNE CO_2 EQUIVALENT)

Fluorinated GHG Group	**2011**	**2012**	**2013**	**2014**	**2015**	**2016**
Fully fluorinated GHGs	42,739,622	29,929,077	23,858,516	27,730,456	24,770,670	39,481,096
Saturated hydrofluorocarbons (HFCs) with 2 or fewer carbon-hydrogen bonds	11,830,986	12,109,647	11,616,289	9,633,496	9,313,549	8,442,867
Saturated HFCs with 3 or more carbon-hydrogen bonds	2,436,833	1,452,855	1,426,863	1,257,906	1,073,521	1,340,253
Saturated hydrofluoroethers (HFEs) and hydrochlorofluoroethers (HCFEs) with 1 carbon-hydrogen bond	23,903	11,913	42,138	98,246	68,548	155,945
Saturated HFEs and HCFEs with 2 carbon-hydrogen bonds	384	555	792	376	319	471
Saturated HFEs and HCFEs with 3 or more carbon-hydrogen bonds	9,262	10,368	9,135	16,090	16,200	33,356
Fluorinated formats	-	-	-	-	-	0
Fluorinated acetates, carbonofluoridates, and fluorinated alcohols other than fluorotelomer alcohols	70	23	96	243	973	829
Unsaturated perfluorocarbons (PFCs), unsaturated HFCs, unsaturated hydrochlorofluorocarbons (HCFCs), unsaturated halogenated ethers, unsaturated halogenated esters, fluorinated aldehydes, and fluorinated ketones	Excluded from analysis	Excluded from analysis	Excluded from analysis	Excluded from analysis	Excluded from analysis	Excluded from analysis
Fluorotelomer alcohols	Excluded from analysis	Excluded from analysis	Excluded from analysis	Excluded from analysis	Excluded from analysis	Excluded from analysis
Fluorinated GHGs with carbon-iodine bond(s)	Excluded from analysis	Excluded from analysis	Excluded from analysis	Excluded from analysis	Excluded from analysis	Excluded from analysis
Other fluorinated GHGs	234,391	169,593	150,352	122,671	166,076	405,231
TOTAL	**57,275,451**	**43,684,030**	**37,104,181**	**38,859,484**	**35,409,856**	**49,860,047**

3A.1.2.4 Container Venting Emissions

Container venting, or container evacuation, is another source of emissions that is common to fluorinated gas production facilities. Emissions from container venting occurred at 6 of the 16 facilities in the U.S. over RY2011 through RY2016. It is anticipated that all container venting emissions are uncontrolled, so no DE assumption is necessary. Table A3.1.6 provides actual GHG emissions for container venting in metric tonne CO_2eq., by individual facility. In later tables, container venting emissions have been included in the emission values along with the emissions from production and transformation processes.

TABLE 3A.1.6 (NEW)
ACTUAL EMISSIONS OF SPECIFIC FLUORINATED GHG FROM CONTAINER VENTING REPORTED UNDER SUBPART L OF THE GHGRP, BY FACILITY (METRIC TONNE AND METRIC TONNE CO_2 EQUIVALENT)

		Tonne						Tonne CO_2eq.					
Facility ID	**Facility name**	**2011**	**2012**	**2013**	**2014**	**2015**	**2016**	**2011**	**2012**	**2013**	**2014**	**2015**	**2016**
526024	3M COMPANY	-	-	-	-	-	-	-	-	-	-	-	-
524391	3M CORDOVA	9	7	-	1	1	3	80,726	65,897	-	11,934	12,237	20,865
527519	3M Cottage Grove Center – Site	-	-	-	-	-	-	-	-	-	-	-	-
526434	ANDERSON DEVELOPMENT COMPANY	-	-	-	-	-	-	-	-	-	-	-	-
526676	ARKEMA, INC.	16	18	15	6	9	10	41,697	61,596	38,772	16,071	23,785	25,096
522460	Chemours - Corpus Christi Plant	-	-	-	-	-	-	-	-	-	-	-	-
523728	CHEMOURS CHAMBERS WORKS	-	-	-	-	-	-	-	-	-	-	-	-
523649	CHEMOURS COMPANY - FAYETTEVILLE WORKS	14	3	6	6	8	8	141,001	29,189	56,284	60,283	72,439	73,468
525649	Chemours EL DORADO	-	-	-	-	-	-	-	-	-	-	-	-
526198	Chemours LOUISVILLE WORKS	-	-	-	-	-	-	-	-	-	-	-	-
523005	Chemours WASHINGTON WORKS	-	-	-	-	-	-	-	-	-	-	-	-
527234	DAIKIN AMERICA INC.	-	-	-	-	-	-	-	-	-	-	-	-
522053	HONEYWELL INTERNATIONAL INC - BATON ROUGE PLANT	-	-	-	-	-	-	-	-	-	-	-	-
522051	HONEYWELL INTERNATIONAL INC - GEISMAR COMPLEX	-	-	-	-	1	-	-	-	-	-	1,494	-
522956	MEXICHEM FLUOR INC.	0	-	-	-	-	-	1	-	-	-	-	-
527776	Versum Materials US, LLC	-	-	-	-	1	-	-	-	-	-	5 ,081	-
	TOTAL	**39**	**28**	**21**	**14**	**20**	**20**	**263,425**	**156,683**	**95,056**	**88,287**	**115,036**	**119,429**

3A.1.2.5 Production and Transformation Quantities Reported Under Subpart OO, Suppliers of Greenhouse Gases

Facilities that produce and transform fluorinated GHGs report the production and transformation quantities to the GHGRP under subpart OO. These data are considered confidential business information on an individual facility basis, and are therefore not publicly available. Table A3.1.7 provides total aggregate fluorinated GHG data on a metric tonne basis for production and transformation processes for subpart OO.

TABLE 3A.1.7 (NEW)
PRODUCTION AND TRANSFORMATION QUANTITIES REPORTED UNDER SUBPART OO OF THE GHGRP (METRIC TONNE)

Quantity	2011	2012	2013	2014	2015	2016
Production and Transformation of Fluorinated Gas	291,000	276,000	302,000	307,000	278,000	315,000

3A.1.3EMISSION FACTOR DEVELOPMENT FOR FLUORINATED GHGS

3A.1.3.1 Estimated pre-abatement emission in metric tonne for Average Emissions Factor Analysis

The average emission factor was developed in terms of metric tonne of emissions. To support this analysis, calculations that estimate the pre-abatement emissions of fluorinated GHG on a metric ton basis must be performed.

The calculations that result in the emissions shown in Table 3A.1.5 above yield GWP-weighted, estimated pre-abatement emissions in metric tonne of CO_2eq. for each production or transformation process. To estimate emissions in metric tonne prior to control, we need a way to estimate the weighted average GWP for each facility and reporting year, to account for the fact that fluorinated GHGs with different GWPs may be controlled at different levels. That is, the GWP distribution of actual emissions may not match the GWP distribution of pre-abatement emissions. We can then divide the emissions in metric tonne of CO_2eq. by the corresponding GWP to calculate the emissions in metric tons. (Recall that the US EPA receives DE range information on a process basis, but does not receive data on individual fluorinated GHGs by process.) The steps we followed to derive the GWPs are outlined below.

a. Weighted-average GWP of controlled emissions. We first calculated the weighted-average GWP of the controlled emissions for each facility and year by dividing (1) the total actual emissions reported by each facility for all production and transformation processes in metric tonne of CO_2eq. by (2) the emissions calculated for each facility in metric tons.[18] However, we cannot necessarily apply this weighted average GWP to the estimated pre-abatement emissions calculated for that facility and year. Because facilities may control emissions with different GWPs to varying extents, the average GWP of the pre-abatement emissions may be different from the average GWP of the actual emissions.

b. Factor to Calculate Weighted-average GWP for Estimated Pre-abatement Emissions. To account for different control levels that may be applied to fluorinated GHGs having different GWPs, we used the process-level reporting of actual emissions by fluorinated GHG group in metric tonne of CO_2eq., as well as our calculations of pre-abatement emissions based on these numbers. Where processes that emit higher-GWP fluorinated GHG groups are controlled to a greater extent than processes that emit lower-GWP fluorinated GHG groups, the calculated emissions of the former will grow more than the calculated emissions of the latter as one moves from the controlled to the pre-abatement scenario. This signal appears in the pre-abatement emissions calculated under the DE assumption in section A3.1.2.3.c above. We can use this signal, along with assumptions about the average GWP of each fluorinated GHG group, to estimate how the weighted-average GWP has changed from the controlled scenario. Using this approach, we developed a ratio of the weighted-average GWP of the estimated pre-abatement emissions to the weighted-average GWP of the actual emissions for each facility and reporting year, and multiplied this ratio by the GWP of the controlled emissions calculated in Step a. Specifically, we performed the following calculations:

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[18] Emissions in metric tonne are calculated as the sum of the emissions that are reported by specific fluorinated GHG in metric tonne (reported in metric tonne of fluorinated GHG), plus the estimated emissions of fluorinated GHGs whose emissions are reported by fluorinated GHG group in metric tonne CO_2eq., after conversion to metric tonne. For the latter, the GWP-weighted emissions are divided by the average GWP for each group to calculate emissions in metric tonne.

1. For each facility and reporting year, we assumed that the emissions of each fluorinated GHG group had the average GWP of that group and divided the metric tonne of CO_2eq. emissions for that group by the weighted-average GWP to obtain estimates of emissions in metric tonne. We then totaled both metric tonne CO_2eq. and metric tonne for all groups, and divided the first by the second to get a weighted-average GWP (uncontrolled) for that facility and year.
2. Then we divided the weighted-average GWP (pre-abatement) for each facility and reporting year by the GWP for the actual controlled scenario for that facility and year to obtain a set of ratios.
3. Finally, we multiplied these ratios by the weighted-average GWPs (for each facility and year) that we calculated for the controlled (actual) scenario in Step a.

The estimated pre-abatement fluorinated GHG emissions, in metric tonne, for production and transformation processes based on the adjusted GWP are provided for the arithmetic mean DE assumption, by individual facility in Table 3A.1.8.

TABLE 3A.1.8 (NEW)
ESTIMATED PRE-ABATEMENT FLUORINATED GHG EMISSIONS FROM PRODUCTION AND TRANSFORMATION PROCESSES PLUS CONTAINER VENTING FROM SUBPART L OF THE GHGRP (USING ARITHMETIC MEAN OF DE RANGE) BY FACILITY (METRIC TONNE)

FACILITY NAME	**2011**	**2012**	**2013**	**2014**	**2015**	**2016**
3M COMPANY	2	4	5	6	2	3
3M CORDOVA	4,348	3,219	2,493	3,005	2,730	4,442
3M Cottage Grove Center – Site	5	7	8	3	3	3
ANDERSON DEVELOPMENT COMPANY	9	9	4			
ARKEMA, INC.	1,018	1,385	1,232	1,075	1,198	1,411
Chemours - Corpus Christi Plant	27	40	35	13	9	35
CHEMOURS CHAMBERS WORKS	75	82	102	73	62	34
CHEMOURS COMPANY - FAYETTEVILLE WORKS	76	68	71	72	109	119
Chemours EL DORADO	22	21	22	22	25	21
Chemours LOUISVILLE WORKS	19	9	12	10		
Chemours WASHINGTON WORKS	297	57	34	29	65	386
DAIKIN AMERICA INC.	44	37	39	44	46	49
HONEYWELL INTERNATIONAL INC - BATON ROUGE PLANT	70	76	78	50	55	41
HONEYWELL INTERNATIONAL INC - GEISMAR COMPLEX	2,547	1,119	1,247	1,243	1,298	430
MEXICHEM FLUOR INC.	42	42	7	7	10	9
Versum Materials US, LLC	39	38	27	26	29	26
TOTAL	**8,638**	**6,211**	**5,415**	**5,680**	**5,641**	**7,009**

3A.1.3.2 Metric of the Emission Factor

The goal of our analysis was to develop an emission factor in terms of metric tonne of fluorinated GHG emissions divided by metric tonne of fluorinated gas produced and transformed (Total emissions in metric tonne / production and transformation quantity produced, in metric tonne). This is because any GWPs or other metrics used to express fluorinated gas emissions relative to CO_2 may go out of date after publication of the emission factor, potentially reducing the applicability of the factor.[19]

We developed an unweighted average EF (i.e., average across facilities of each facility's emission factor, where that factor equals the facility's emissions divided by the sum of that facility's production and transformation). We also examined the standard deviation of the facility-specific emission factors. For an average, each facility is weighted equally and facilities with comparatively larger or smaller EF values influence the average value even if the quantities that they produce and/or transform are small. The average emission factor, based on an average, was calculated to be 0.04 metric tonne fluorinated GHG emissions per metric tonne quantity produced and transformed.

TABLE 3A.1.9 (NEW)
DEFAULT EMISSION FACTOR FOR FLUORINATED PRODUCTION

	2011	2012	2013	2014	2015	2016	Average Across Years
EF based on Arithmetic Mean, metric tonne/ metric tonne	0.05	0.04	0.03	0.04	0.03	0.04	0.04
Standard Deviation	0.1	0.1	0.07	0.1	0.08	0.1	
Relative Standard Deviation	200%	250%	230%	250%	270%	250%	
95% confidence interval	390%	490%	450%	490%	520%	490%	470%

3A.1.4ANALYSIS OF COMMON FLUORINATED GHGS EMITTED FROM FLUOROCHEMICAL PROCESSES

The emission factor in Table A3.1.9 is expressed in terms of metric tonne emitted per metric tonne produced or transformed. To be of use for an emissions inventory, knowledge of, or assumptions regarding, the fluorinated GHGs emitted is necessary. This section summarizes the data and approach used for identifying the most emitted fluorinated GHGs from fluorochemical production based on the data reported by facilities to the U.S. GHGRP.

3A.1.4.1 Develop Ratios for Most Emitted Fluorinated GHG Emissions Analysis

To identify the most emitted fluorinated GHGs, the analysis begins with comparing the actual emissions by fluorinated GHG group (summarized in Table A3.1.3) with the estimated pre-abatement emissions (the estimated pre-abatement emissions are shown in Table A3.1.5). The DE range is provided for each production and transformation process but is not provided for individual specific fluorinated GHGs. To calculate these pre-abatement emissions, we need a way to estimate the unweighted metric tonne for each fluorinated GHG group and reporting year. The calculations in Table A3.1.5 yield GWP-weighted, pre-abatement emissions in metric tonne CO_2eq. for each production or transformation process. A ratio of the pre-abatement emissions in metric tonne CO_2eq. compared to the actual emissions in metric tonne CO_2eq. can be developed for each fluorinated GHG group and reporting year. These ratios can then be applied to the actual emissions of specific fluorinated GHG in metric tonne CO_2eq. to appropriately estimate the pre-abatement level of specific fluorinated GHG in metric tonne. (Recall that the US EPA does not receive data on unweighted emissions, metric tonne, of individual fluorinated GHGs by process.) The ratios of pre-abatement metric tonne CO_2eq. compared to actual metric tonne CO_2eq. are provided in Table A3.1.10.

A3.1.4.2 Pre-abatement Emissions in metric tonne CO_2eq. and metric tonne for Specific Fluorinated GHGs, for Production and Transformation Processes, and Container Venting

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[19] We also reviewed factors using GWP-weighted emissions and production/transformation quantities because they provided insight into how the GWPs of fluorinated GHGs emitted relate to the GWPs of fluorinated gases produced across facilities.

Applying the ratios in Table A3.1.10 to the Table A3.1.2 actual emissions provides the pre-abatement emissions by fluorinated GHG (in metric tonne CO_2eq.). The ratios were multiplied by the specific fluorinated GHG, based on its fluorinated GHG group, for each reporting year. The estimated pre-abatement emissions by specific fluorinated GHG, in metric tonne CO_2eq. and metric tonne, are provided in Table A3.1.11 for production and transformation processes, along with the container venting emissions.

A3.1.4.3 Representative Fluorinated GHG Profile

The most commonly emitted fluorinated GHGs on a pre-abatement emissions basis can be determined from the data set. The most common fluorinated GHGs, by metric tonne and by metric tonne CO_2eq., are shown in Table A3.1.12. Those fluorinated GHGs that do not have GWPs in any IPCC Assessment Report (e.g., the Fifth Assessment Report) have been dropped from the list (i.e., hexafluoropropylene oxide, and octafluorotetrahydrofuran). The analysis shows the representative chemical composition in metric tonne for the top 10 fluorinated GHGs.

TABLE 3A.1.10 (NEW)
RATIOS OF ESTIMATED PRE-ABATEMENT EMISSIONS IN METRIC TONNE CO_2 EQUIVALENT (USING ARITHMETIC MEAN OF DE RANGE) TO ACTUAL EMISSIONS IN METRIC TONNE OF CO_2 EQUIVALENT

Fluorinated GHG Group	2011	2012	2013	2014	2015	2016
Fully fluorinated GHGs	15.9	11.5	7.2	12.9	12.8	22.5
Saturated hydrofluorocarbons (HFCs) with 2 or fewer carbon-hydrogen bonds	2.9	2.8	2.9	3.6	4.2	6.1
Saturated HFCs with 3 or more carbon-hydrogen bonds	3.6	2.3	2.2	2.5	2.2	2.7
Saturated hydrofluoroethers (HFEs) and hydrochlorofluoroethers (HCFEs) with 1 carbon-hydrogen bond	7.2	3.5	1.7	2.3	1.6	1.6
Saturated HFEs and HCFEs with 2 carbon-hydrogen bonds	5.5	191.2	193.2	198.0	6.7	7.0
Saturated HFEs and HCFEs with 3 or more carbon-hydrogen bonds	2.5	2.5	1.9	4.3	3.9	6.3
Fluorinated formats						1.6
Fluorinated acetates, carbonofluoridates, and fluorinated alcohols other than fluorotelomer alcohols	1.1	1.4	1.0	1.0	8.1	6.6
Unsaturated perfluorocarbons (PFCs), unsaturated HFCs, unsaturated hydrochlorofluorocarbons (HCFCs), unsaturated halogenated ethers, unsaturated halogenated esters, fluorinated aldehydes, and fluorinated ketones	Excluded from analysis	Excluded from analysis	Excluded from analysis	Excluded from analysis	Excluded from analysis	Excluded from analysis
Fluorotelomer alcohols	Excluded from analysis	Excluded from analysis	Excluded from analysis	Excluded from analysis	Excluded from analysis	Excluded from analysis
Fluorinated GHGs with carbon-iodine bond(s)	Excluded from analysis	Excluded from analysis	Excluded from analysis	Excluded from analysis	Excluded from analysis	Excluded from analysis
Other fluorinated GHGs	5.8	4.9	3.8	4.7	6.1	5.9

TABLE 3A.1.11 (NEW)
ESTIMATED PRE-ABATEMENT FLUORINATED GHG EMISSIONS FROM PRODUCTION PROCESSES, TRANSFORMATION PROCESSES, AND CONTAINER VENTING FROM SUBPART L OF THE GHGRP (USING ARITHMETIC MEAN OF DE RANGE), BY SPECIFIC FLUORINATED GHG (METRIC TONNE CO_2 EQUIVALENT AND METRIC TONNE)

Fluorinated GHG Name	2011	2012	2013	2014	2015	2016	Sum Total, tonne	2011	2012	2013	2014	2015	2016	Sum Total, tonne CO_2eq.
PFC-14 (Perfluoromethane)	961	882	417	605	581	1,224	4,670	7,099,740	6,517,927	3,082,715	4,471,865	4,293,330	9,047,657	34,513,233
HFC-134a	780	621	599	731	963	904	4,598	1,115,275	888,437	857,188	1,045,203	1,377,357	1,292,344	6,575,805
Perfluorocyclobutane	846	404	188	372	359	1,169	3,338	8,717,609	4,161,124	1,932,044	3,829,822	3,700,681	12,038,028	34,379,308
HFC-32	452	459	436	418	551	556	2,872	305,085	309,916	294,328	281,876	371,685	375,472	1,938,362
HFC-125	447	428	450	543	579	387	2,834	1,565,149	1,496,910	1,574,237	1,901,966	2,025,422	1,355,484	9,919,168
HFC-23	556	596	567	403	341	322	2,784	8,227,363	8,814,039	8,386,194	5,960,713	5,047,891	4,763,628	41,199,828
HFC-143a	492	299	290	249	201	274	1,805	2,199,566	1,337,071	1,295,696	1,111,496	899,663	1,223,588	8,067,080
Nitrogen trifluoride	493	322	141	204	194	286	1,639	8,472,427	5,534,029	2,420,335	3,510,222	3,331,771	4,921,716	28,190,500
Hexafluoropropylene oxide	197	201	143	260	305	411	1,517	1,969,139	2,005,481	1,427,557	2,604,466	3,054,522	4,109,247	15,170,411
PFC-116 (Perfluoroethane)	327	232	287	219	297	40	1,402	3,991,281	2,827,549	3,498,551	2,674,161	3,625,619	484,819	17,101,979
Octafluorotetrahydrofuran	301	290	285	299	72	108	1,355	3,005,532	2,901,350	2,848,074	2,993,494	715,725	1,084,733	13,548,907
Pentafluoro(trifluoromethyl)-cyclopropane	164	95	74	145	245	343	1,065	1,640,970	945,229	743,174	1,445,947	2,449,359	3,429,930	10,654,610
PFC-218 (Perfluoropropane)	202	89	346	211	42	63	953	1,785,524	783,260	3,058,038	1,859,967	373,114	557,703	8,417,605
PFC-5-1-14 (Perfluorohexane, FC 72)	187	94	57	132	162	135	769	1,741,556	877,250	532,641	1,227,637	1,508,328	1,260,091	7,147,504
HFC-245fa	173	112	109	124	90	110	718	178,341	115,212	112,576	127,561	93,150	112,998	739,839
HFC-227ea	76	70	100	85	108	138	578	245,039	226,497	321,319	274,773	347,144	444,859	1,859,631
Trifluoromethyl sulphur pentafluoride	123	108	135	67	34	38	505	2,176,556	1,906,677	2,394,848	1,187,441	607,481	668,577	8,941,579
HFE-449sl, (HFE-7100) Isomer blend	27	28	23	39	34	68	219	7,899	8,194	6,890	11,646	10,205	20,154	64,987
PFC-3-1-10 (Perfluorobutane)	32	17	44	34	13	48	188	284,753	153,082	392,867	296,961	116,592	422,942	1,667,196
Perfluorodiethyl ether	27	34	15	18	21	36	151	267,613	337,690	154,228	175,707	209,907	364,894	1,510,039
HFC-152a	32	21	27	0	0	57	137	3,915	2,656	3,355	0	0	7,023	16,949
PFC-4-1-12 (Perfluoropentane)	33	10	7	8	22	33	114	302,372	94,043	65,179	76,544	199,003	306,266	1,043,407
Sulphur hexafluoride	20	13	23	38	13	6	113	462,400	294,817	529,256	864,085	295,614	132,818	2,578,990
2H-perfluoro(5-methyl-3,6-dioxanonane)	23	22	12	8	14	32	111	45,291	44,616	23,279	16,442	28,198	64,653	222,479

TABLE 3A.1.11 (NEW) (CONTINUED)
ESTIMATED PRE-ABATEMENT FLUORINATED GHG EMISSIONS FROM PRODUCTION PROCESSES, TRANSFORMATION PROCESSES, AND CONTAINER VENTING FROM SUBPART L OF THE GHGRP (USING ARITHMETIC MEAN OF DE RANGE), BY SPECIFIC FLUORINATED GHG (METRIC TONNE AND METRIC TONNE CO_2 EQUIVALENT)

Fluorinated GHG Name	**2011**	**2012**	**2013**	**2014**	**2015**	**2016**	**Sum Total, tonne**	**2011**	**2012**	**2013**	**2014**	**2015**	**2016**	**Sum Total, tonne CO_2eq.**
Trifluoromethanesulfonyl fluoride	19	21	23	18	10	8	99	38,164	41,308	46,446	35,632	19,053	16,439	197,043
Pentafluoro(trifluoromethoxy)-ethane	31	12	21	13	7	11	96	307,788	123,664	212,517	130,809	73,289	108,866	956,934
Hexafluorooxetane	22	11	25	8	9	14	89	222,031	107,999	253,398	84,905	90,084	135,633	894,051
1,1,1,2,2,3,3-Heptafluoro-3-(1,2,2,2-tetrafluoroethoxy)-propane	3	2	6	15	10	24	61	21,710	11,216	41,875	98,125	67,150	155,716	395,791
Perfluorobutanesulfonyl fluoride	7	4	4	4	8	30	57	14,158	8,234	7,949	8,739	16,279	59,609	114,969
HFC-236fa	7	9	14	10	8	9	57	64,409	92,657	136,907	102,260	76,647	90,648	563,528
PFC-6-1-12	18	15	1	2	4	0	39	141,418	115,806	7,764	14,326	28,302	0	307,616
2,2,3,3,4-Pentafluoro-4-(trifluoromethyl)-oxetane	5	10	12	5	2	2	36	49,625	100,763	117,861	47,284	19,511	22,941	357,986
Carbonyl fluoride	9	4	3	4	5	7	32	17,338	8,230	5,092	8,564	9,703	14,629	63,556
Trifluoroacetyl Fluoride	7	4	3	4	5	6	28	14,520	8,132	5,089	7,778	10,115	11,091	56,727
Perfluoro-2-(2-Fluorosulfonylethoxy) Propyl Vinyl Ether	0	0	0	0	7	17	23	0	0	0	0	13,276	33,186	46,462
Perfluoropropionyl fluoride	6	4	4	3	5	0	22	11,228	8,170	8,592	5,117	9,915	0	43,022
HFC-43-10mee	3	3	3	3	0	6	17	4,819	4,186	4,780	4,172	0	9,354	27,311
isobutyryl fluoride	14	0	0	0	0	0	14	27,191	0	0	0	0	0	27,191
Unknown FC	0	0	0	0	3	9	12	0	0	0	0	28,910	87,380	116,291
Heptafluoropropyl Trifluoromethyl Ether	2	1	2	0	1	5	12	20,717	11,513	22,341	0	14,576	46,882	116,029
Perfluro compounds, C5-18	0	0	0	1	0	9	10	0	0	281	10,799	0	90,662	101,741
1,1,1,3,3,5,5,7,7,9,9,11,11-tridecafluoro-2,4,6,8,10-pentaoxadodecan-12-oyl fluoride	0	0	0	0	9	0	9	0	0	0	0	18,330	0	18,330
HFC-365mfc	0	0	7	0	0	0	7	0	0	5,894	0	0	0	5,894
Unknown Sulfonated FC	0	0	2	1	0	3	6	0	0	22,629	13,366	0	27,823	63,818
2,3,3,3-Tetrafluoro-2-(trifluoromethoxy)propionyl fluoride	3	3	0	0	0	0	6	6,643	5,785	0	0	0	0	12,429
HFC-227ca	0	1	3	0	0	0	4	0	3,117	7,792	0	0	12	10,921
2-Butene, 2-chloro-1,1,1,3,4,4,4-heptafluoro	4	0	0	0	0	0	4	8,038	0	0	0	0	0	8,038

TABLE 3A.1.11 (NEW) (CONTINUED)
ESTIMATED PRE-ABATEMENT FLUORINATED GHG EMISSIONS FROM PRODUCTION PROCESSES, TRANSFORMATION PROCESSES, AND CONTAINER VENTING FROM SUBPART L OF THE GHGRP (USING ARITHMETIC MEAN OF DE RANGE), BY SPECIFIC FLUORINATED GHG (METRIC TONNE AND METRIC TONNE CO_2 EQUIVALENT)

Fluorinated GHG Name	**2011**	**2012**	**2013**	**2014**	**2015**	**2016**	**Sum Total, tonne**	**2011**	**2012**	**2013**	**2014**	**2015**	**2016**	**Sum Total, tonne CO_2eq.**
1H-perfluorooctane	0	0	0	0	0	4	4	0	0	0	0	0	14,703	14,703
C5F13N	2	0	0	0	1	0	4	24,634	0	0	0	13,454	0	38,088
[[Difluoro(trifluoromethoxy)methoxy] difluoromethoxy] difluoro-acetyl fluoride	0	0	0	0	0	3	3	0	0	0	0	0	6,987	6,987
C6F15N	3	0	0	0	0	0	3	32,227	0	0	0	0	0	32,227
Propanenitrile, 2,3,3,3-tetrafluoro-2-(trifluoromethyl)-	0	0	0	0	0	3	3	0	0	0	0	0	6,406	6,406
Perfluorotributyl amine	2	1	0	0	0	0	3	18,802	12,132	0	0	0	0	30,934
Trifluoroacetic Acid	0	0	3	0	0	0	3	0	0	5,239	0	0	0	5,239
C6F12	0	0	0	0	1	0	1	0	0	0	0	12,944	0	12,944
C7F16O	0	0	1	0	0	0	1	0	0	10,613	0	0	0	10,613
2,3,3,3-Tetrafluoro-2-(heptafluoropropoxy)propanoyl fluoride	0	0	0	0	0	0	1	0	0	0	0	741	466	1,207
Perfluroisobutyric acid fluoride	0	0	0	0	0	0	0	0	0	0	0	0	442	442
1,1,1,3,3,3-hexafluoropropane	0	0	0	0	0	0	0	0	0	0	0	0	91	91
2,2,3,3,4,4,-hexafluoro-4-(fluorosufonyl)-butanoyl fluoride	0	0	0	0	0	0	0	0	0	0	0	0	39	39
Oxetane, 2,2,3,4,4-Pentafluoro-3-(trifluoromethyl)-	0	0	0	0	0	0	0	0	0	0	0	0	156	156
1,2-Oxathiane, 3,3,4,4,5,5,6,6-octafluoro-, 2,2-dioxide	0	0	0	0	0	0	0	0	0	0	0	0	6	6
Propanoyl fluoride, 2,2,3,3-tetrafluoro-	0	0	0	0	0	0	0	0	0	0	0	0	5	5
HFC-236ea	0	0	0	0	0	0	0	0	0	0	0	0	3	3
TOTAL	**7,137**	**5,551**	**4,914**	**5,303**	**5,338**	**6,958**	**35,202**	**56,855,857**	**43,245,968**	**36,877,626**	**38,521,874**	**35,204,040**	**49,429,797**	**260,135,162**

TABLE 3A.1.12 (NEW)
TOP-10 EMITTED SPECIFIC FLUORINATED GHG, FROM PRODUCTION PROCESSES, TRANSFORMATION PROCESSES, AND CONTAINER VENTING FROM SUBPART L OF THE GHGRP (USING ARITHMETIC MEAN OF DE RANGE ENDPOINTS)[A]

Fluorinated GHG Name	Sum total, tonne	Percent	GHG Group
PFC-14 (Perfluoromethane)	4,670	18%	Fully fluorinated GHGs
HFC-134a	4,598	18%	Saturated HFCs with 2 or fewer carbon-hydrogen bonds
Perfluorocyclobutane	3,338	13%	Fully fluorinated GHGs
HFC-32	2,872	11%	Saturated HFCs with 2 or fewer carbon-hydrogen bonds
HFC-125	2,834	11%	Saturated HFCs with 2 or fewer carbon-hydrogen bonds
HFC-23	2,784	11%	Saturated HFCs with 2 or fewer carbon-hydrogen bonds
HFC-143a	1,805	7%	Saturated HFCs with 3 or more carbon-hydrogen bonds
Nitrogen trifluoride	a	a	Fully fluorinated GHGs
Hexafluoropropylene oxide	b	b	Fully fluorinated GHGs
PFC-116 (Perfluoroethane)	1,402	5%	Fully fluorinated GHGs
Octafluorotetrahydrofuran	b	b	Fully fluorinated GHGs
Pentafluoro(trifluoromethyl)-cyclopropane	b	b	Fully fluorinated GHGs
PFC-218 (Perfluoropropane)	953	4%	Fully fluorinated GHGs
PFC-5-1-14 (Perfluorohexane, FC 72)	769	3%	Fully fluorinated GHGs

Due to rounding, the sum of individual items will not equal 100%.

[a] The *2019 Refinement* includes separate emission factors specifically for NF_3 production. As approximately 92 percent of NF_3 emissions are from intended NF_3 production, and NF_3 is not commonly emitted from the production of other fluorochemicals, NF_3 has been dropped from the analysis for representative composition.

[b] These fluorinated GHGs that do not have GWPs in any IPCC Assessment Report (e.g., the Fifth Assessment Report) have been dropped from the analysis for representative composition.

3A.1.5 UNCERTAINTY ANALYSIS OF AVERAGE EMISSION FACTOR

In addition to examining the sensitivity of calculated uncontrolled (i.e., pre-abatement) emissions to various assumptions regarding the DE, we performed a Monte Carlo analysis to comprehensively assess the uncertainty of the emission factor, given the uncertainty of the DE as well as other sources of uncertainty. The uncertainty in the estimated pre-abatement emission in units of metric tonne CO_2eq. is based on the wide ranges of the DE. The uncertainty in the pre-abatement emission estimates in terms of metric tonne of fluorinated GHG is based on the combination of the uncertainty in the DE and the uncertainty in the average GWP of the specific fluorinated GHGs in the pre-abatement scenario. With respect to the DEs, we used the following assumed distribution.

TABLE 3A.1.13 (NEW)
DISTRIBUTION ASSUMPTIONS FOR THE DE RANGES

DE ranges	Distribution Assumptions
≥0% to <75%	Half of the values are 0%; half of the values flat distribution between 0 and 74.9%
≥75% to <95%	Flat distribution between 75 and 94.9%
≥95% to <99%	Flat distribution between 95 and 98.9%
≥99%	Triangular distribution between 99 and 99.99% with mode at 99%

Because we expected that a significant number of reporters using the ≥0 to <75 percent range were uncontrolled, we assumed a distribution function that assigns half of the distribution function to 0 percent DE.

For estimating the uncertainty in the GWP, we evaluated the data for emissions by specific fluorinated GHG compound (in metric tonne of specific GHG) that was reported for the facility as a whole. We developed different GWP distributions for each facility and fluorinated GHG group combination based on the data reported for a given facility. If only one specific fluorinated GHG compound was reported for a given facility within a fluorinated GHG group (or if all of the specific GHGs reported by the facility were identical), the GWP of that compound was used directly (no uncertainty). If multiple specific fluorinated GHG compounds with different GWPs were reported within a fluorinated GHG group for a given facility, we calculated the weighted average GWP for that group based on the specific fluorinated GHG's GWP and direct mass emissions reported by that facility. The weighted average GWP across all reporting years was used as the central tendency value and the weighted average for individual years was used to assess the range of the distribution function for the uncertainty analysis. In some cases, the emissions for specific fluorinated GHG compounds in a group did not exceed the separate reporting threshold (1,000 metric tonne CO_2eq.) of subpart L, and only the metric tonne CO_2eq. emissions for the fluorinated GHG group were reported at the facility level. In this case, the individual GWPs for all compounds listed within that fluorinated GHG group was used as the distribution function, and a random GWP was selected from those values. When we first utilized this approach, the very low-GWP fluorinated GHG groups (i.e., those groups whose members had GWPs near or below 1) dominated the estimated pre-abatement fluorinated GHG emissions (in direct mass terms), which led to huge uncertainties in the mass emission rates for compounds that had a negligible impact on emissions in terms of CO_2eq. Consequently, we excluded the very-low-GWP fluorinated GHG groups' emissions when estimating the mass of fluorinated GHG compound emissions for developing the proposed emissions factor. For similar reasons, we used a lower GWP of 0.5 for the fluorinated acetates, carbonofluoridates, and fluorinated alcohols other than fluorotelomer alcohols group, rather than 0.05 value for 4,4,4-trifluorbutan-1-ol (CAS No. 461-18-7). It was assumed that, even if this compound was the primary pollutant emitted from this group, small amounts of other compounds from this group would also likely be emitted and that the value of 0.5 was a reasonable lower bound for this group.

Calculations of the pre-abatement emissions (in both metric tonne CO_2eq. and in metric tonne of fluorinated GHG group) were made using the process level emissions reported under subpart L. A Monte Carlo analysis using 10,000 random realizations was used to estimate the average and 95th percentile confidence intervals for the emissions. We assumed the uncertainty in the reported production quantities were negligible relative to the uncertainties in the uncontrolled emissions.

The average annual estimated pre-abatement emissions in metric tonne CO_2eq. from the Monte Carlo analysis compares reasonably well with but are slightly lower than the pre-abatement emissions estimates using the arithmetic mean DE assumption for the range. This is because the lowest and highest DE ranges were skewed towards the lower DE values in the Monte Carlo analysis. The total estimated pre-abatement emissions in metric tonne of fluorinated GHG compounds from the Monte Carlo analysis (when excluding the low GWP groups) had similar uncertainty ranges as the total estimated pre-abatement emissions in CO_2e (which are based only on uncertainty of the DE) for most facilities. A few facilities that had reported generic emissions of the fluorinated acetates, carbonofluoridates, and fluorinated alcohols other than fluorotelomer alcohols group had much higher uncertainty in their mass emissions than in their CO_2e emissions due to the variability and uncertainty associated with the GWP.

The uncertainty in the average emission factor across all of the reporting facilities (i.e., the 95-percent confidence interval around the sample mean), including the uncertainties in both the DE and in the GWP of the emitted gases, was 20 percent. In summary, these sources of uncertainty are mitigated by the large number of data points in the analysis, which come from the large number of processes and significant number of years covered. Thus, the errors related to the DE estimated for each individual process and to the mix of gases emitted tend to balance out, and the aggregate uncertainty is reduced.

It is important to note that the uncertainty in the emission factor for any single facility is much larger than this, and is dictated by the fact that true pre-abatement emission rates naturally vary from facility to facility depending on the fluorochemicals produced and the processes used to make them. This variability appears in the U.S. EPA data as differences in the estimated pre-abatement emission factors across facilities, differences that persist over the entire time series. The year-to-year variability seen in the estimated pre-abatement emission factor for any one facility is generally much smaller than this facility-to-facility variability. The uncertainty shown in Table 3A.1.9 reflects this variation among facilities. The 95 percent confidence interval (calculated based on the relative standard deviation among the facilities' emission factors) is ±470 percent. Because there cannot be a negative emission factor on the low side, a value of 0.001 was selected as the lower uncertainty bound, as it is representative of lower emission factor values seen in the data set. This results in an uncertainty range for the Tier 1 default emission factor of 0.001 to 0.2.

As noted in section 3A.1.2 above, the selected EF is based on the straight average analysis. The average EF based on the straight average is similar to the EF based on the Monte Carlo analysis. The overall EF that results from other assumptions, such as use of a weighted average or use of the geometric mean, are also provided in Table 3A.1.14 to provide additional context.

TABLE 3A.1.14 (NEW)
COMPARISON OF EMISSION FACTOR VALUES IN PARALLEL ANALYSES

Selected EF	**EF value, metric tonne/metric tonne**
Arithmetic Mean DE assumption, straight average	**0.04**
Other EF Bases	
Arithmetic Mean DE assumption, weighted average	0.02
Geometric Mean DE assumption, weighted average	0.05
Monte Carlo	0.04

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