

CHAPTER 3

CHEMICAL INDUSTRY EMISSIONS

[Parts shaded in grey – the unchanged text from the 2006 IPCC Guidelines]

Second-order Draft**Authors****Section 3.1**

Jochen Harnisch (Germany)

Sections 3.2 – 3.8

Charles Jubb (Australia)

Alexander Nakhutin (Russia) and Virginia Carla Sena Cianci (Uruguay)

Sections 3.3

Retno Gumilang Dewi (Indonesia) María José López Blanco (Spain)

Section 3.9

Robert Lanza (USA)

Thomas Martinsen (Norway), Abdul Karim W. Mohammad (Iraq), and Maruo M. O. Santos (Brazil)

Section 3.10

Archie McCulloch (UK) and Brian T. Mader (USA)

Sections 3.10

Karen S. Schaffner (USA), Deborah A. Ottinger (USA) and Brian T. Mader (USA)

Sections 3.11

Håkon Frøysa Skullerud (Norway), Katsuhiko Hirose (Japan) and Samir Tantawi (Egypt)

Contributing Authors**Sections 3.2 – 3.8**

Javier Pérez-Ramírez (Spain)

Section 3.9

Maarten Neelis (Netherlands) and Martin Patel (Germany)

Sections 3.10

Jeffrey B. Coburn (USA) and Gregory M. Watson (USA)

Sections 3.11

Richard Chahine (Canada), Shohei Oyama (Japan) and Nigel Brandon (UK)

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3 CHEMICAL INDUSTRY EMISSIONS

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

[This section, 3.3.2.2, is an update of section 3.3.2.2 Chapter 3 Volume 3 of *2006 IPCC Guidelines* and should be used instead of the section 3.3.2.2 Chapter 3 Volume 3 of 2006 IPCC Guidelines.]

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 N₂O 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 N₂O, and associated uncertainties.

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

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TABLE 3.3A (NEW) DIFFERENT PLANT TYPES FOR THE PRODUCTION OF HNO3 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 N₂O 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 ₂ O Emission Factor (relating to 100 percent pure acid)
Old (pre-1975) plants* (all processes)	10-19 kg N ₂ O/tonne nitric acid ^a
Single low pressure plants	5 kg N ₂ O/tonne nitric acid ±10%
Single medium pressure plants	8 kg N ₂ O/tonne nitric acid ±20% ^b
Single high pressure plants	9 kg N ₂ O/tonne nitric acid ±40%
Single pressure plants with abatement technology**	2.5 kg N ₂ O/tonne nitric acid ±10% ^b
Dual Pressure (M/H)	9 kg N ₂ O/tonne nitric acid ±30% ^b
Dual Pressure (M/H) with abatement technology	2.5 kg N ₂ O/tonne nitric acid ±20% ^b
Dual Pressure (L/M)	7 kg N ₂ O/tonne nitric acid ±20% ^b
Dual Pressure (L/M) with abatement technology	1.5 kg N ₂ O/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 it is still operating. ** Applies to all single pressure plants using all levels of N ₂ O abatement measures (primary, secondary, tertiary and quaternary). These abatement measures include all levels of abatement such as process-integrated abatement technologies, tailgas N ₂ O destruction and non-selective catalytic reduction (NSCR, a NO _x abatement technology that can also be managed to abate N ₂ O). Source: ^a Based on IPCC, 2000; EC, 2007; and the tests from CDM projects presented in USEPA, 2010. ^b Based on information from EC, 2007; EC, 2009; 2017 Annex I Party GHG Inventory Submissions; and Joint Implementation projects available at the UNFCCC web-site.	

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TIER 3 METHOD

Plant measurements provide the most rigorous data for calculating net emissions (i.e., N₂O generation and destruction factors). Monitoring N₂O 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 N₂O, 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

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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

This section, 3.10.1.2, is an update/elaboration of section 3.10.1.2 Chapter 3 Volume 3 of 2006 IPCC Guidelines and should be used instead of the section 3.10.1.2 Chapter 3 Volume 3 of the *2006 IPCC Guidelines*.

To remain consistent with the updated terminology in section 3.10.2, the terminology used for the Tier 3 method in this section has been updated to refer to the development and use of an “emission factor method” rather a “proxy method.” In addition, the lower bound emission factor presented for optimised plants has been updated to reflect the value that appeared in the final, published paper.

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.

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

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

Where:

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

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

$P_{\text{HCFC-22}}$ = 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 (UNCHANGED)**TIER 2 CALCULATION OF HFC-23 FROM HCFC-22 (PRODUCED) USING FACTOR(S) CALCULATED FROM PROCESS EFFICIENCIES**

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

Where:

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

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

$P_{\text{HCFC-22}}$ = 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 (UNCHANGED)**CALCULATION OF HFC-23 EMISSION FACTOR FROM CARBON BALANCE EFFICIENCY**

$$EF_{\text{carbon_balance}} = \frac{(100 - \text{CBE})}{100} \cdot F_{\text{efficiency loss}} \cdot \text{FCC}$$

Where:

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

CBE = carbon balance efficiency, percent

$F_{\text{efficiency loss}}$ = 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

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EQUATION 3.33 (UNCHANGED)**CALCULATION OF HFC-23 EMISSION FACTOR FROM FLUORINE BALANCE EFFICIENCY**

$$EF_{\text{fluorine_balance}} = \frac{(100 - FBE)}{100} \cdot F_{\text{efficiency loss}} \cdot FFC$$

Where:

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

FBE = fluorine balance efficiency, percent

$F_{\text{efficiency loss}}$ = 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 (UNCHANGED)**TIER 3A CALCULATION OF HFC-23 EMISSIONS FROM INDIVIDUAL PROCESS STREAMS (DIRECT METHOD)**

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

Where:

$E_{\text{HFC-23}}$ = 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**

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

Where:

$E_{\text{HFC-23}}$ = total HFC-23 emissions: E_{ij} 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 (UNCHANGED)**TIER 3C CALCULATION OF HFC-23 EMISSIONS FROM INDIVIDUAL PROCESS STREAMS
(BY MONITORING REACTOR PRODUCT)**

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

Where:

$E_{\text{HFC-23}}$ = 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 (UNCHANGED)**TIER 3A CALCULATION OF 'INSTANTANEOUS' HFC-23 EMISSIONS IN AN INDIVIDUAL PROCESS
STREAM (DIRECT METHOD)**

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

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 datum 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.

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

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

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**

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

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 m³/hour of feedstock)

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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 (UNCHANGED)**TIER 3C CALCULATION OF HFC-23 EMISSIONS FROM AN INDIVIDUAL FACILITY BY IN-PROCESS MEASUREMENT**

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

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.

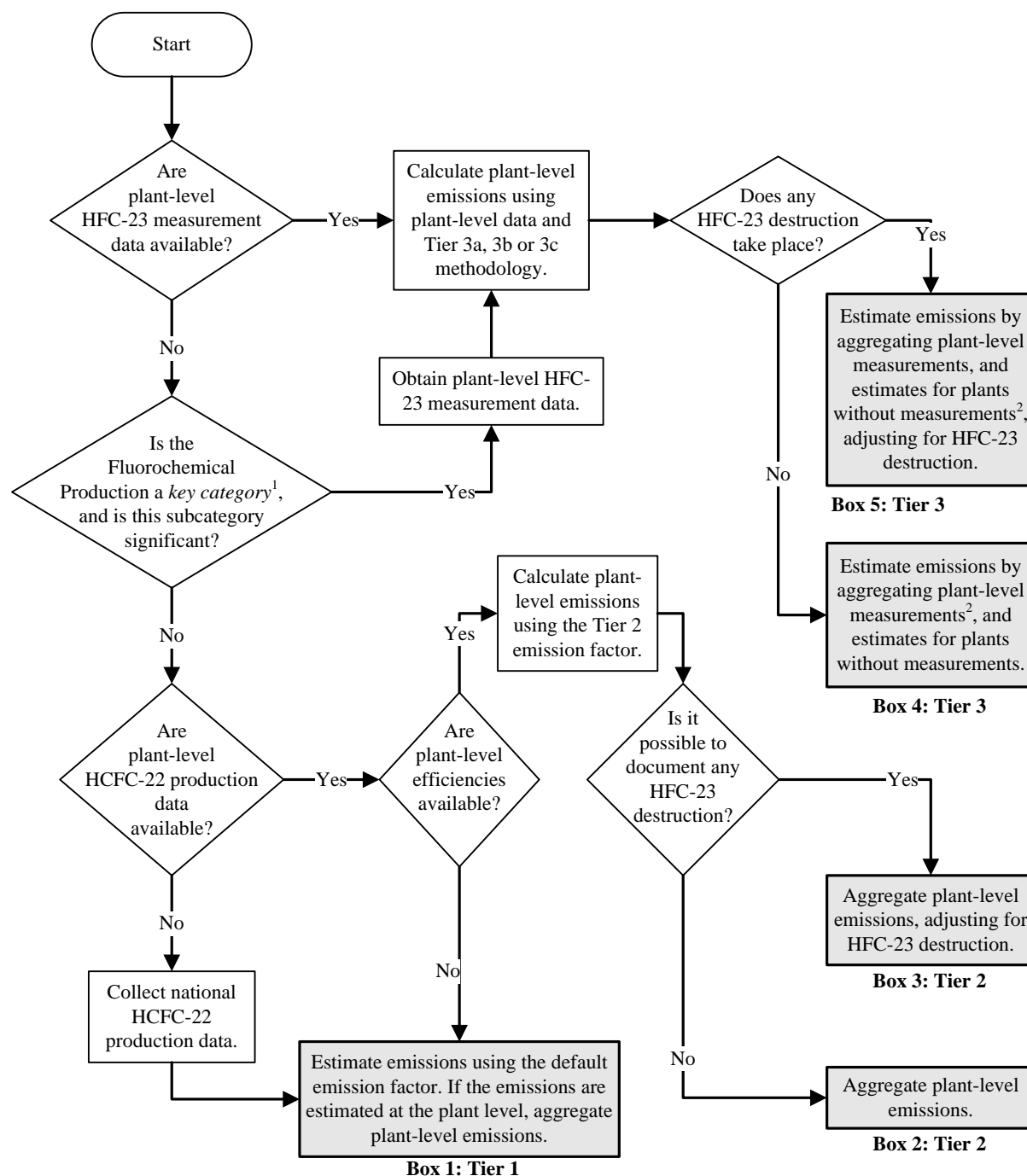
The total quantity of HFC-23 released into the atmosphere is the sum of the quantities from the individual release periods and individual reaction systems.

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.

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Figure 3.16(unchanged) 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; USEPA, 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. An average emission factor of 0.019 has been reported for “business as usual” operations; for new operations located in developing countries that operate without significant abatement, the emission factor is 0.04 (McCulloch, 2007). 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
<i>For comparison:</i>	
<i>Optimised large plant- requiring measurement of HFC-23 (Tier 3)</i>	<i>Down to 0.015</i>
<i>Plant with effective capture and destruction of HFC-23 (Tier 3)</i>	<i>Down to zero</i>

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 (UNCHANGED)
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

[This section, 3.10.1.3, is an update/elaboration of section 3.10.1.3 Chapter 3 Volume 3 of 2006 IPCC Guidelines and should be used instead of the section 3.10.1.3 Chapter 3 Volume 3 of 2006 IPCC Guidelines

This section has been updated to refer to the “emission factor method” rather than the “proxy method.”]

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

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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

This section, 3.10.2.1, is an update/elaboration of section 3.10.2.1 Chapter 3 Volume 3 of 2006 IPCC Guidelines and should be used instead of the section 3.10.1.2 Chapter 3 Volume 3 of 2006 IPCC Guidelines

This section has been updated to clarify the full range of emissions and their sources at fluorochemical production plants.

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-products emissions. For example, in a national inventory for a fluorochemical plant, significant by-product emissions of SF₆, CF₄, C₂F₆, C₃F₈, C₄F₁₀, C₅F₁₂ and C₆F₁₄ were reported (UNFCCC, 2005). Other examples include the release of by-product N₂O and CF₄ from the production of NF₃ (Tasaka, 2004; 2007), CF₄ from the production of CFC-11 and 12, or of SF₆ 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 processes²:

- Telomerization Process used in the production of fluorochemicals fluids and polymers
- Photooxidation of tetrafluoroethylene to make fluorochemical fluids
- Direct Fluorination often used in SF₆ production
- Halogen Exchange Processes to make low boiling PFCs like C₂F₆ and CF₄, HFC 134a and 245fa
- NF₃ manufacturing by direct fluorination
- Production of uranium hexafluoride
- Production of fluorinated monomers like tetrafluoroethylene and hexafluoropropylene
- Production of fluorochemical agrochemicals

² This list is illustrative.

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- Production of fluorochemical anesthetics
- Production of perfluoropolyethers
- Production of hydrofluoroolefins (HFO) such as tetrafluoropropene and its precursors

Halogen exchange processes are extensively used for HFC manufacture, while most PFCs and SF₆ 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 CoF₃. 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 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. 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 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. Further enquiries (see Figure 3.17) can then elucidate whether or not there are significant fluorochemical greenhouse gas emissions.

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

This section, 3.10.2.2, is an update/elaboration of section 3.10.2.2 Chapter 3 Volume 3 of 2006 IPCC Guidelines and should be used instead of the section 3.10.2.2 Chapter 3 Volume 3 of 2006 IPCC Guidelines

This section has been updated and elaborated. Guidance for the Tier 3 method now includes a method to estimate emissions from equipment leaks and more detail to the method for estimating emissions from process vents. New default emission factors are presented for the Tier 1 method.

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. EPA 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, SF₆ and other fluorinated greenhouse gases. The default emission factors in Table 3.29a are expressed in terms of kg emitted/kg produced).

EQUATION 3.41 (UNCHANGED) 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

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EF_{default, k} = default emission factor, kg/kg

P_k = total production of fluorinated greenhouse gas *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 and SF₆ 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. 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 speciation 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, the Tier 2 estimate is further improved.

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

$$E_k = \sum_i \sum_j \int_t C_{ijk} \bullet M_{ij} \quad [\int_t \text{ means the quantity should be summed over time.}]$$

Where:

E_k = total 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 and concentrations *C* 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. 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 where emissions are summed over all streams *j*, all equipment types *g*, at all plants *i*, over a given time period *t*.

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 process vent and equipment leak production-related emissions of fluorinated greenhouse gas *k*.

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E_{kPV} = total process vent, production-related emissions of fluorinated greenhouse gas k .

E_{kEL} = total equipment leak, production-related emissions of fluorinated greenhouse gas k .

Process vent and equipment leaks are described as follows:

Process Vents

Process vents are typically configured for frequent 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**

$$E_{kPV} = \sum_i \sum_j \int_t C_{ijk} \cdot f_{ijk} \quad \left[\int_t \text{ means the quantity should be summed over time.} \right]$$

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 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 3.35 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**

$$E_{kPV} = \sum_i \sum_j \int_t E_{ijk} \quad \left[\int_t \text{ means the quantity should be summed over time.} \right]$$

Where:

E_{kPV} = total production-related emissions of fluorinated greenhouse gas k :

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

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 Tier 3 approach includes 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 U.S. EPA (1995): the screening ranges approach, correlation approach, and unit-specific correlation approach.

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

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from U.S. EPA (1995) for many types of equipment (these U.S. 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 U.S. 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**

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

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 U.S. EPA (1995).

CE_g = exponent for correlation equation for equipment type g .

SV_{igk} = 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.

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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 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.

$$\text{EQUATION 3.43C (NEW)}$$

$$\text{TIER 3 CALCULATION OF A UNIT-SPECIFIC CORRELATION}$$

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

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.

β_1 = slope of regression equation.

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

$$\text{EQUATION 3.43D (NEW)}$$

$$\text{TIER 3 CALCULATION OF EMISSIONS FROM EQUIPMENT LEAKS USING A UNIT-SPECIFIC CORRELATION APPROACH}$$

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

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.

$SBCF$ = Scale bias correction factor (The $SBCF$ is a function of the mean square error of the correlation in log space, as described in USEPA (1995).

C_{ijk} = 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 .

$$\text{EQUATION 3.43E (NEW)}$$

$$\text{TIER 3 CALCULATION OF PRODUCTION-RELATED EMISSIONS FROM PROCESS VENTS USING A SITE- OR PROCESS-SPECIFIC EMISSION FACTOR}$$

$$E_{kEL} = \sum_i \sum_j \sum_k \int_t E_{gijkEL} \quad [\int_t \text{ means the quantity should be summed over time.}]$$

Where:

E_{kEL} = total equipment leak, production-related emissions of fluorinated greenhouse gas k :

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.

Should values of E_{L-ijgk} originate from the Unit-Specific Correlation approach, special care must be used to ensure that these E_{L-ijgk} are used only for the particular equipment type and plant where they were generated.

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CHOICE OF EMISSION FACTORS**Process Emissions**

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. 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 1 relies on default emission factors. 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. For Tier 1, the default emission factors in Table 3.28a assume there is no use of abatement, and these default emission factors include emissions from both process vents and equipment leaks (Schaffner et. al. 2018). 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.

TABLE 3.28A (NEW) TIER 1 DEFAULT EMISSION FACTOR FOR FLUOROchemical PRODUCTION	
Emission Factor (kg fluorinated GHG emissions/kg fluorochemical produced) ^{a, b}	Uncertainty for default emission factor for fluorochemical production
0.04	-98% to +470% (0.001 to 0.2)
Source: ^a EPA 2017a, EPA 2017b. ^b Schaffner et. al. 2018	

The default emission factor listed in Table 3.28a was estimated using data from U.S. EPA 2017a and 2017b, described in detail by Schaffner et. al. (2018). 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 U.S. EPA has data. For each facility, the emission factors for each year were then averaged over the six years of reporting, and the resulting averages for each facility 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 provides a universal default emission factor that is applicable where the manufacturing method is likely unknown, as is often the case in a Tier 1 calculation. As noted above, emission rates from different manufacturing methods can vary widely, a pattern seen in the variation of the emission factors across the reporting facilities. 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.

A variety of fluorinated GHGs can be emitted from fluorochemical manufacturing processes other than the compounds 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. To derive this composition, six years of U.S. EPA GHGRP data were sorted, and the chemical species with the highest estimated uncontrolled emissions (in metric tons) were identified. The weighted average GWP of these emissions is the same as the weighted average GWP of the uncontrolled

³ Fluorochemicals produced in the U.S. and reported to the GHGRP include HFCs, HFEs, PFCs, SF₆, NF₃, 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.

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emissions (other than very low-GWP emissions) estimated for fluorinated gas producers that report to the U.S. EPA.⁴

TABLE 3.28B (NEW)	
REPRESENTATIVE CHEMICAL COMPOSITION OF THE EMITTED MASS	
Fluorinated GHG emitted	Percentage emitted (% of unweighted tons)
HFC-134a	17
PFC-14 (Perfluoromethane)	17
Perfluorocyclobutane	12
HFC-32	11
HFC-125	11
HFC-23	10
HFC-143a	7
Nitrogen trifluoride	6
PFC-116 (Perfluoroethane)	5
PFC-218 (Perfluoropropane)	4
Source:	
^a EPA 2017a, EPA 2017b.	
^b Schaffner et. al. 2018b	

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 SF₆ produced in Germany, an emission factor of 0.002 of the total quantity of SF₆ produced was found for facilities whose customers do not require highly purified SF₆ gas (e.g., electrical equipment, insulated windows) (Preisegger, 1999). However, it is not known whether the 0.002 factor is based on pre-abatement emissions or controlled, post-abatement emissions, and therefore it should not be used for Tier 1 estimates. For SF₆ produced in Japan, a factor of 0.08 was found for facilities whose customers require highly purified SF₆ 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 SF₆ emission factor has been reported as 0.03 of sales (O’Connell 2002). U.S. and Japanese NF₃ manufacturers have reported an emission factor for NF₃ emissions of 0.02 in 2009, with a goal of eventually achieving an emission factor of 0.005 (it is not known whether these factors are based on pre-abatement emissions or controlled, post-abatement emissions) (Fthenakis, 2010). CF₄ and N₂O are generated as a by-product during NF₃ manufacture, N₂O and CF₄ can be formed at rates of 0.03 and less than 0.01, respectively, relative to the mass of NF₃ formed during electrolysis (these emission factors are on an uncontrolled, pre-abatement basis) (Tasaka, 2004; 2007). If national data are available, these should be used, particularly for other materials not specifically listed here. 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. When the inventory compiler has enough plant-specific information (e.g., process knowledge that confirms whether the higher or lower emission factors should be used, or knowledge of the specific fluorinated GHGs that coincides with the fluorinated GHGs named above in the text), it would be appropriate to use these fluorinated GHG specific factors. When less is known about the plant and processes, it is *good practice* to use the default emission factor in Table 3.28a.

Emission Control Technology

The default emission factors (Tier 1) are based on situations where no abatement measures are employed. For Tiers 2 and 3, 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. Based on the experience in the destruction of HFC-23, a default destruction efficiency of 100 percent is suggested. As an example, when a thermal oxidation 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,

⁴ To develop both the mass emission factor in Table 3.29A and the break-out of fluorinated GHGs in Table 3.29B, EPA included fluorinated GHGs with GWPs above one. 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 tons of CO₂e emitted/ton produced.

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976 in the case of a treatment system with 99 percent removal efficiency, the magnitude of fluorinated GHG emissions
977 would be dominated by the amount of process uptime.

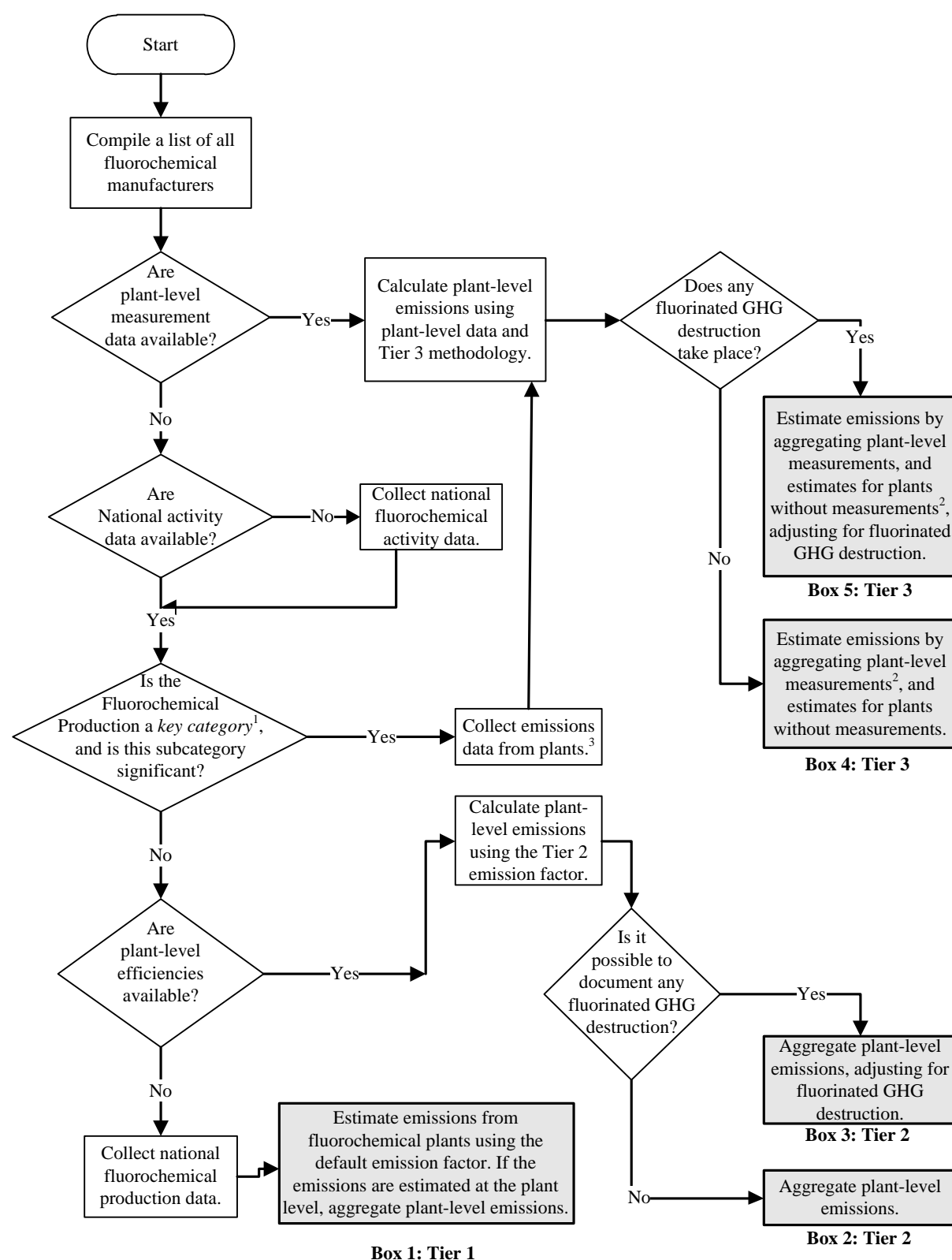
978 Emission control technologies are used at many facilities to control fluorinated GHG emissions from process vents.
979 Destruction and removal efficiencies (DREs) are generally based on performance testing of emission control
980 devices. Results are expected to vary across process equipment and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

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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.

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CHOICE OF ACTIVITY DATA

Again, activity data has no role in the Tiers 3 and 2 estimates, which are based on measurements. For Tier 1, the activity is the annual mass of the desired fluorochemical that is produced.

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

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

This section, 3.10.2.3, is an update/elaboration of section 3.10.2.3 Chapter 3 Volume 3 of the 2006 IPCC Guidelines and should be used instead of the section 3.10.2.3 Chapter 3 Volume 3 of 2006 IPCC Guidelines.

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 U.S. 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 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 is the exact extent to which the emissions from individual processes are controlled by the facilities reporting to the U.S. 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%.

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

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1054 produce a much larger uncertainty than that from Tier 3, the utility of Tier 2 is likely to be limited to assessing
1055 whether or not by-product fluorochemical emissions are a significant subcategory under *key category*.

1056 **3.10.2.4 QUALITY ASSURANCE/QUALITY CONTROL (QA/QC),**
1057 **REPORTING AND DOCUMENTATION**

1058 No Refinement

1059

3.11 HYDROGEN PRODUCTION

[This section, 3.11, is a new section in the Chapter 3 Volume 3 of the *2019 Refinement*. It should be placed after section 3.10 Chapter 3 Volume 3 of the *2006 IPCC Guidelines*.]

This Section describes methodological guidance for Hydrogen production when it is produced as a pure main product at a stand-alone facility.

Hydrogen can also be produced as a by-product or intermediate product at Refineries, Ammonia, Methanol and other Chemical process industries. 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 2 Energy or Volume 3 IPPU. Emissions from production of hydrogen as part of mixtures with other gases, e.g., syngas, are not covered by this section.

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

3.11.1 Introduction

The dominating hydrogen production technologies, accounting for more than 95 % of the global hydrogen production, are steam reforming and gasification of fossil fuels (Ogden 1999, Speirs et al. 2017). These 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 hydrogen. When hydrogen is the final product (see Box 3.15), a series of enhancement and purification steps yields a highly pure hydrogen output (99.999% purity is normal at present). The remaining production is mainly done by electrolysis of water. Other production methods are biological technologies, like fermentation and photo biological water splitting, electrolytic technologies, photo catalytic technologies and thermolysis. Efforts have been made to increase the carbon free hydrogen production by developing new technologies, and a development in low emission methods is expected. However, methods using fossil input materials are currently dominating due to economic reasons (Speirs et al. 2017).

Technologies for hydrogen production might generate process and/or combustion emissions of greenhouse gases (GHGs), or no direct GHG emissions at all (i.e. no emissions at the production facility). Only production methods generating process GHG emissions from fossil feedstocks should be considered in this sector. Emissions from combustion should be included only if the fuel is derived from the feedstock in an integrated production process. If a separate fuel is used, the GHGs from the fuel combustion should be estimated by methods provided in Vol. 2, Ch. 2 and reported under sector 1 Energy (stationary combustion). Emissions of CO₂ from thermochemical processes like steam reforming and gasification using biomass as feedstock should be accounted for in a memo item, and not included in national totals. Production methods generating no direct GHG emissions, like electrolysis of water, should not be considered in the IPPU sector.

Hydrogen may be produced as a pure main product (Box 3.15) at stand-alone facilities, or it may be produced as a by-product for sale or an intermediate product in f. ex. refineries, ammonia, methanol or other chemical factories. Only emissions from production of hydrogen as a pure main product at stand-alone facilities should be reported in this sector. Where hydrogen is produced as a by-product for external use or as an intermediate product, the emissions are typically already accounted for in the emission estimates for the respective sectors derived using methodological guidance in Volume 2 Energy or Volume 3 IPPU. For instance, intermediate hydrogen production in refineries is covered in Volume 2 Energy (fugitive emissions). Where hydrogen is produced as a by-product for external use or as an intermediate product in industries other than mentioned above (refineries, ammonia and methanol), it is *good practice* to estimate emissions from hydrogen production by using the methodological guidance in Volume 3 IPPU (hydrogen production or ammonia production) that minimises uncertainties in the national inventory, and to transparently note which method(s) are used. Double counting should be avoided. The emissions from the hydrogen production should be allocated to the current source category (i.e. the category where the emissions occur).

If the resolution of activity data may not enable separate estimates to be made for the production of pure main product hydrogen, it is important to ensure that there are no gaps or double-counts in the emission estimates presented in the Energy and IPPU sectors. National circumstances may therefore determine whether to report emissions from by-product or intermediate hydrogen production in the Hydrogen Production sector or in the sector of the main product (e.g., Refineries or Ammonia Production). It is *good practice* to estimate and report emissions from hydrogen production in ways that minimise uncertainties in the national inventory and to transparently note where emissions from hydrogen production are included (fully or in part) within Energy and/or other IPPU source categories. See Box 3.16 for details about double counting.

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For hydrogen produced inside of an end use process, for instance in a vehicle fuel cell using methanol or hydrocarbons as input materials, the emissions should be reported in the sector of the end use. Hydrogen can also be embedded into organic hydrides to facilitate the transport to the end users (see Box 3.17). The chemical process releasing hydrogen at the end user produces no process emissions of GHGs. Accordingly, where fossil fuels are combusted to heat the reaction, the resulting CO₂ emissions should be allocated to the Energy sector (stationary combustion).

Some hydrogen production methods generate GHGs as an unintended constituent of the product. For instance, hydrogen produced by biological processes might 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 product itself or from the combustion of it, and should be estimated by methods provided in the guidance for the sector of the end user (i.e. not in the hydrogen production sector) and reported in that sector.

Steam reforming and gasification produce CO₂ emissions and very minor emissions of methane and N₂O. However, only CO₂ should be estimated from hydrogen production, as emissions of methane and N₂O are very low and the literature evidence is insufficient to establish an estimation method. Hence no reporting of methane and N₂O is required in this sector (see Box 3.18).

Summary of current hydrogen production methods and the allocation of emissions to sector are shown in Table 3.29.

BOX 3.15 (NEW)
DEFINITIONS

Pure hydrogen and gas mixtures

Pure hydrogen is hydrogen gas purified to meet industry product quality standards. Hydrogen not defined as pure are defined gas mixtures. Pure hydrogen is produced by complete oxidation technologies or other technologies (Table 3.29). Gas mixtures, e.g. syngas, are produced by technologies partially oxidising the feedstock.

Final products and intermediate products

A final product is the intended output product(s) 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 product 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, fuel and input material

Feedstock is the total input material in a manufacturing process. Raw material is the part of the feedstock being transformed into the final 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). Input material includes both fuel from separate sources and feedstock.

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

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

Notes:

¹ 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 2 Energy or Volume 3 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.

² Biogenic emissions are reported as a memo item (i.e. not included in the IPPU totals) and non-biogenic emissions are reported to IPPU.

³ No process emissions, as the feedstock does not contain carbon. All emissions arise from combustion of fuels to power the production process.

⁴ Only direct emissions (i.e. emissions generated in the production facilities during production) are considered, according to standard IPPU methodology.

⁵ 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, emissions from production of hydrogen reported in the **Hydrogen production sector** must be excluded from other sectors. Conversely, 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 hydrogen is produced as a by-product or intermediate product, e.g. in oil refining (Energy) or in ammonia or methanol production (IPPU), the emissions are typically already accounted for in the emission estimates for the respective sectors derived using methodological guidance in Volume 2 Energy (fugitive emissions) or Volume 3 IPPU.
- Where hydrogen is produced as a by-product for external use or as an intermediate product in industries other than the three mentioned above, it is *good practice* to estimate emissions from hydrogen production by using the methodological guidance in Volume 3 IPPU (ammonia, methanol, hydrogen or current sector) that minimises uncertainties in the national inventory, and to transparently note which method(s) are used. Double counting should be avoided. The emissions from hydrogen production should be allocated to the source category where the emissions occur.
- If the resolution of activity data does not enable separate estimates to be made for the hydrogen production, it should be ensured that no gaps or double-counts in the emission estimates are presented in the Energy and IPPU sectors. Hence, national circumstances may determine whether to report emissions from by-product or intermediate hydrogen production in the Hydrogen Production sector or in the Sector of the main product (e.g., Refineries, Ammonia or Methanol Production).
- Emissions from fuel being derived from the feedstock should be reported in the same sector as the process emissions. Emissions from fuel provided from external sources should be reported in Energy sector (stationary combustion). A more detailed description is given in Vol. 3 IPPU, Chapter 1.2.1.
- Recovered CO₂ might be delivered for downstream use, for instance as raw material in other production processes or as dry ice (cooling, cleaning, etc.), or sent to permanent storage. It is *good practice* to report the emission of CO₂ from downstream use in the **downstream sector**, and to subtract the recovered CO₂ from the Hydrogen production sector. If the emission from use of recovered CO₂ is reported in the downstream sectors, but the recovery is not subtracted from the CO₂ emissions in the Hydrogen production sector, a double-count will occur. Conversely, if the emission the downstream sector is not reported but the recovery is subtracted from the emissions in the Hydrogen production sector, a gap will occur.
- If the downstream emission is not reported in the corresponding sectors, the recovered amount should be reported as emission (i.e. not subtracted) in the **Hydrogen production** sector. In certain cases, it may prove difficult to verify whether the recovered CO₂ is used in downstream sectors or not. In such cases, a sound consideration should be made whether to report the recovered CO₂ as emission the Hydrogen production sector or not. The downstream use and permanent storage should be transparently described.
- It is *good practice* to estimate and report emissions from hydrogen production in ways that minimise uncertainties in the national inventory and to transparently note where emissions from hydrogen production are included (fully or in part) within Energy and/or other IPPU source categories. A transparent description should be given.

Box 3.17 (NEW)**ORGANIC HYDRIDES USED AS HYDROGEN CARRIERS**

Hydrogen can be reacted with aromatic substances like benzene and toluene at a hydrogen production facility to form liquid organic hydrides. These liquids are transported to a hydrogen filling station where the hydrogen is released by a chemical reaction and filled into f. ex. a vehicle. The reaction releasing hydrogen produces no process emission of GHGs. However, the organic hydride is converted back to the original aromatic substance and transported to the production facility for embedding 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 CO₂ should be allocated to the Energy sector (stationary combustion).

BOX 3.18 (NEW)**METHANE AND N₂O EMISSIONS FROM HYDROGEN PRODUCTION**

Based on current literature evidence, it is not practicable to develop methods for estimation of emissions of methane and N₂O from hydrogen production; evidence is scarce on methane and N₂O emission sources for many production technologies, activity data for the process combustion source are likely to be hard to obtain, and current evidence indicates that methane emission levels are likely to be very low.

Emissions of methane and N₂O from the production of hydrogen include *fugitive emissions* of methane from valves, flanges, storage and transfer, etc. and emissions from *combustion* of fuel to produce heat for the reforming process. However, the literature is very scarce regarding the fugitive emissions. Furthermore, the combustion of fuel is an integrated part of the production process, in which the fuel is derived from the feedstock. The activity data for the combustion might therefore be difficult to obtain, as well as the emissions being very low (see for example EFs for combustion in Vol. 2, Table 2.3).

Minor amounts of methane might be produced in the production process as well; at present a maximum of 2% is reported in some anaerobic biological methods (Braga et al 2017). However, these methods produce hydrogen in a closed anaerobic atmosphere, from which no direct emissions can occur, and hence the methane will be part of the product and should not be reported as emissions in the hydrogen sector, or alternatively the methane is removed in a purification step and used as fuel in the production process. In the case of biological production methods, which do not power the reactions by fuel combustion, these are currently not widespread in a commercial scale and literature describing emissions from these processes is very scarce.

Establishing methods for estimation emissions of methane and N₂O from hydrogen production is therefore considered impractical at this stage, as evidence to develop methods is insufficient, activity data might be very uncertain, and the emissions are considered very low. If literature evidence becomes available, establishing estimation methods for methane and N₂O should be considered in a future update or refinement of the *IPCC Guidelines*.

BOX 3.19 (NEW)**USES OF HYDROGEN**

Hydrogen (H₂) is a gas with similar flammable properties as natural gas and gasoline (Hydrogen Council 2017). The main uses of hydrogen at present 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 system in renewable electricity production, as main constituent in coal gas (city gas) used for heating and cooking, and in semiconductor industry processing and welding. Combustion or conversion of hydrogen to produce heat and electricity yields zero carbon dioxide emissions. An increase in the use of hydrogen is expected in near future, due to an increase in low-carbon technologies.

This section describes methods to estimate emissions from hydrogen *production*. These emissions are independent of how hydrogen is being used. However, where CO₂ is recovered in the Hydrogen production sector the end use should be estimated and reported in the respective sector to allow for subtraction (Box 3.16).

3.11.2 Methodological issues

The most widespread methods for hydrogen production at present are, by far, steam reforming and gasification of fossil feedstocks. Both technologies oxidise the feedstock during the process itself and in combustion to heat the process. Oxidation of fossil feedstocks generates CO₂, and efforts are made to develop alternative methods with no (or reduced) CO₂ emissions. At present, most of these technologies are at an experimental level, while some are mature and commercially available in an industrial scale (f. ex. electrolysis of water).

Technologies for producing hydrogen from fossil or biogenic feedstocks 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 (Table 3.29). Complete oxidation technologies convert all feedstock carbon into CO₂ (except a small residue of solid carbon), and they have hydrogen as the main product. The CO₂ emissions can be

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estimated quite easily from feedstock consumption or hydrogen production data. Partial oxidation technologies convert parts of feedstock carbon into CO₂, and they result in gas mixtures having hydrogen as a constituent. In several industries using hydrogen as a raw material, partial oxidation technologies are often used to produce an intermediate mixture of hydrogen and CO (syngas, Box 3.21), as also CO is needed for raw material. To regulate the H₂:CO ratio hydrogen might be separated from the mixture as a by-product and burnt for fuel or used externally (e.g. sold).

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 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 an external energy source, 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. If the feedstock is biogenic, the CO₂ should be reported in a memo item and not be included in the national totals. Waste may contain both fossil and biogenic materials. The same applies to fossil fuels with biofuel mixed in. The CO₂ emissions from feedstocks containing a mix of fossil and biogenic carbon should be allocated partly to the hydrogen sector and partly to a memo item, relative to the respective fossil and biogenic carbon shares.

In both the hydrogen producing reactions (overall) and the combustion reaction there is a close to 1:1 molar relation between the produced CO₂ 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

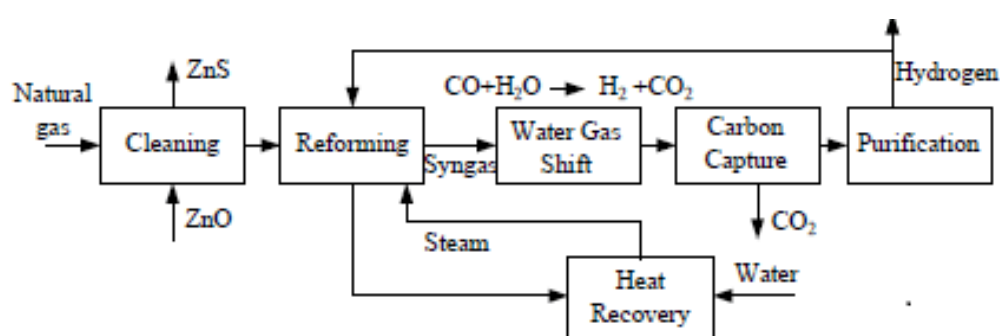
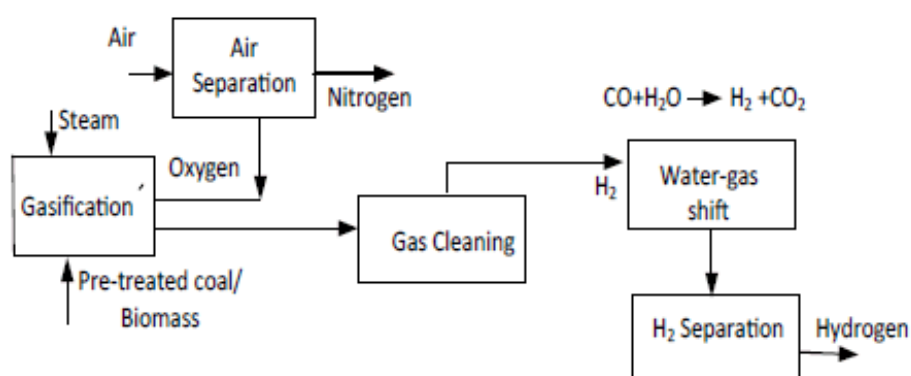


Figure 3.19 (new) Hydrogen production via gasification with water gas shift reaction¹



Note:

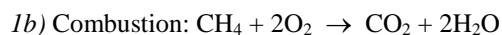
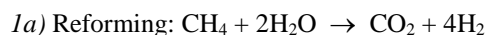
¹ The flue gas from the H₂ separation step, containing CO and methane, is burnt in a boiler to produce heat (i.e. steam).

Source:

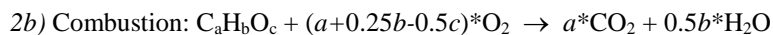
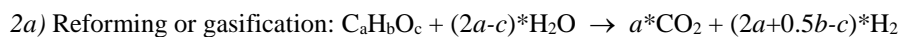
Madzen et al. (2015), The National Energy Technology Laboratory (2017).

Box 3.20 (NEW)**CHEMICAL REACTIONS IN HYDROGEN PRODUCTION BY COMPLETE OXIDATION TECHNOLOGIES**

Steam reforming of natural gas (overall reactions):

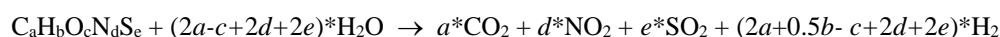


Steam reforming or gasification of other fossil or biogenic feedstocks (overall general formulas):

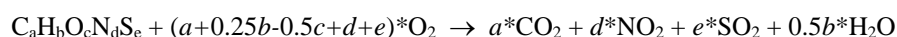


Gasification of waste (overall general formulas):

3a) Gasification:



3b) Combustion:



In all these overall reactions the consumed feedstock carbon atoms to produced CO_2 molecules ratio 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. The output gas mixture is called syngas (Box 3.21).

Emissions from syngas production are not covered by the estimation methods in this section, as syngas is not a pure hydrogen product. However, emissions from syngas intermediate and hydrogen by-product production in refineries, ammonia, methanol and other industrial production are covered in the respective sectors.

Box 3.21 (NEW)**SYNGAS**

Syngas is a gas mixture containing hydrogen, carbon monoxide and sometimes smaller amounts of CO₂, 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, including steam reforming, gasification, partial oxidation and autothermal reforming, in the presence of heat. The feedstock is 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. From the syngas surplus hydrogen might be separated out and purified into a by-product to obtain a proper H:CO ratio in the syngas. Emissions from syngas production are not covered by the estimation methods in this section, as syngas is not a pure hydrogen product. Instead, emissions from syngas intermediate and hydrogen by-product production in refineries, ammonia, methanol and other chemical production are covered in the respective 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

Production of hydrogen by water electrolysis is widespread, mainly in small-scale plants, and accounts for about 4 % of current global hydrogen production. Other methods for hydrogen production are currently at a minor or experimental level. Several of the methods, e.g. water electrolysis and photo induced water splitting, are without direct GHG emissions. Others, e.g. steam reforming of ammonia and thermal water splitting, have no process emissions of GHGs but emissions arising from stationary combustion of fuels to heat the production process, and accordingly these emissions are allocated to the energy sector.

Biological methods including fermentation produce hydrogen by using living microbes like algae and bacteria. In the production process either fossil or biogenic fuels are consumed under anaerobic conditions, and the output products are hydrogen containing minor amounts of CO₂, methane and other organic substances, and CO₂ off-gas. Biological methods are still in a very small-scale use, and parts of the CO₂ off-gas are captured by the microbes. Methane and other GHGs being produced are parts of the product and 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.

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 1a, 2a and 3a methods are based on feedstock data, while the Tier 1b, 2b and 3b methods are based on hydrogen production data. The Tier 1c method is based hydrogen production data on a total national or regional level, or production capacity if production data are not available. Note that *emissions arising from production of hydrogen in refineries, ammonia, methanol and other industries (i.e. intermediates or by-products) is included in the respective sectors and should be excluded from the hydrogen production sector*, to avoid double counting (c.f. Box 3.16). Where emissions of GHGs arise from production of intermediate or by-product hydrogen (incl. gas mixtures containing hydrogen) in sectors not provided with a methodology for estimating these emissions it is *good practice* to use either of the methodological approaches in Volume 3 IPPU (ammonia, methanol or hydrogen) that minimise uncertainties in the national inventory, and to transparently note which methods are used. Double counting should be avoided. The emissions from hydrogen production should be allocated to the current source category (i.e. the category where the emissions occur).

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 a method has a lower uncertainty than the Tier b method at the same Tier level. The Tier 1c method has the highest uncertainty.

Emissions from fuel combustion should be reported in the Hydrogen production sector insofar the fuel is consumed as an integrated part of the production process, i.e. taken from the feedstock. Otherwise it should be reported in the energy sector.

If the feedstock is biogenic, the CO₂ emission should be allocated to a memo item and not included in national totals. If the feedstock contains both fossil and biogenic components (e.g., biodiesel, waste, etc.), the CO₂ emission

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should be allocated partly to the hydrogen sector and partly to the memo item, relative to the respective fossil and biogenic carbon shares.

Recovered CO₂ is typically delivered for downstream use in other manufacturing industries, but it could also be used in on-site production or sent to permanent storages. The CO₂ recovered for use as input material in downstream manufacturing processes, for example dry ice used in freezing applications, will most often be emitted to the atmosphere in the respective manufacturing industry or during use of the manufactured product. It is *good practice* to subtract recovered CO₂ from the estimated emissions in the Hydrogen production sector and to include the emissions in the respective downstream sectors. If the recovered CO₂ is sent to permanent storage, it is *good practice* to subtract the recovered CO₂ from the Hydrogen production sector and to document such storage. If the emissions are not reported in the respective downstream sectors and/or permanent storage of the CO₂ cannot be documented, it is *good practice* to not subtract these recovered amounts from the CO₂ emissions. See Box 3.16 for more details.

Feedstock data reported in mass units or volume units need to be converted into energy units (GJ) before estimating emissions.

TIER 1 METHOD

The Tier 1 methods use *national or regional level activity data* together with *default factors* and data on recovered CO₂ 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 1a) or production of hydrogen (Tier 1b and 1c). In the Tier 1a 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 1c method total national or regional activity data and the general default factors in Table 3.30 could be used.

The CO₂ emissions are estimated as follows:

EQUATION 3.44 (NEW)
CO₂ EMISSIONS FROM HYDROGEN PRODUCTION – TIER 1A

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

EQUATION 3.45 (NEW)
CO₂ EMISSIONS FROM HYDROGEN PRODUCTION – TIER 1B

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

EQUATION 3.46 (NEW)
CO₂ EMISSIONS FROM HYDROGEN PRODUCTION – TIER 1C

$$E_{co_2} = HP \bullet FRF \bullet CCF \bullet \frac{44}{12}$$

Where:

E_{CO2} = emissions of CO₂ (tonnes)

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

HP = pure hydrogen produced as main product (tonnes)

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} = CO₂ recovered (tonnes)

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 tonnes, conversion can be done by using the default

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calorific values in the Ch. 1, Vol. 1 of *2006 IPCC Guidelines*⁵. 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 1c method. Double counting with other sectors should be avoided (Box 3.16). 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 CO₂ (see Section 3.11.2.2 for details).

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 national totals. If the biogenic part cannot be estimated, it is *good practice* to assume that all feedstock is fossil. If no data on recovered CO₂ 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.

TIER 2 METHOD

The Tier 2 methods use *national or regional level activity data* together with *country specific factors* and data on recovered CO₂ 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 CO₂ emissions are estimated as follows:

EQUATION 3.47 (NEW)
CO₂ EMISSIONS FROM HYDROGEN PRODUCTION – TIER 2A

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

EQUATION 3.48 (NEW)
CO₂ EMISSIONS FROM HYDROGEN PRODUCTION – TIER 2B

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

Where:

E_{CO_2} = emissions of CO₂ (tonnes)

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 (tonnes)

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_{CO_2} = CO₂ recovered (tonnes)

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_j s 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 CO₂ (see Section 3.11.2.2 for details).

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 national totals. A fuel containing a fossil and a biogenic part should be split

⁵ For plastic gasification the NCV value is given in the footnote to Table 3.30.

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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, 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 CO₂ and stored amounts of carbon to derive emissions. The CO₂ emissions are estimated as follows:

$$\begin{aligned} &\text{EQUATION 3.49 (NEW)} \\ &\text{CO}_2 \text{ EMISSIONS FROM HYDROGEN PRODUCTION – TIER 3A} \\ &E_{co_2} = \sum_{j,n} (FC_{j,n} \bullet CCF_{j,n} \bullet 44/12) - (R_{co_2} + S_c \bullet 44/12) \end{aligned}$$

$$\begin{aligned} &\text{EQUATION 3.50 (NEW)} \\ &\text{CO}_2 \text{ EMISSIONS FROM HYDROGEN PRODUCTION – TIER 3B} \\ &E_{co_2} = \sum_{i,j,n} (HP_{i,j,n} \bullet FRF_{i,j,n} \bullet CCF_{j,n} \bullet 44/12) - (R_{co_2} + S_c \bullet 44/12) \end{aligned}$$

Where:

E_{CO_2} = emissions of CO₂ (tonnes)

$FC_{i,j,n}$ = 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* (tonnes)

$FRF_{i,j,n}$ = 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_{CO_2} = CO₂ recovered (tonnes)

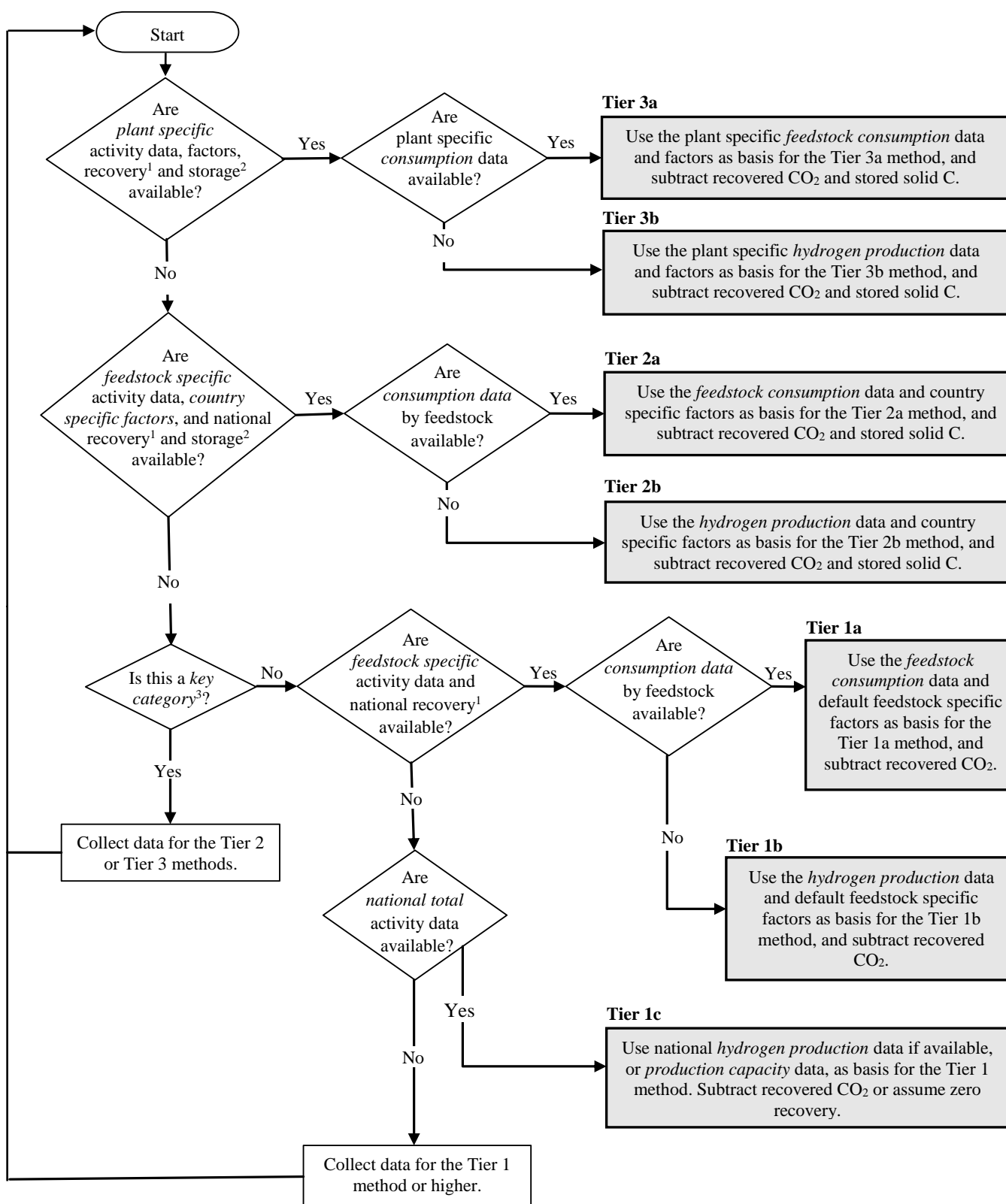
S_c = stored solid carbon (tonnes)

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 national totals. Fuels containing a fossil and a biogenic part should be split according to the respective fossil and biogenic carbon shares.

Stored 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 carbon is available, it is *good practice* to assume that it is pure carbon. It is *good practice* to exclude stored carbon from the estimated emissions in the hydrogen production sector. In the Hydrogen production sector, stored carbon does not include recovered CO₂ 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 CO₂ emissions from hydrogen production

Note:

¹ Recovery = annual mass of CO₂ 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 tonnes of carbon.

TIER 1 METHOD

In the Tier 1 a method, it is *good practice* to use the default feedstock specific CCFs in Table 3.30, and in the Tier 1b 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 1c 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 REQUIREMENTS AND CARBON CONTENT FACTORS FOR HYDROGEN PRODUCTION^{1,2}

Production Process	Feedstock requirement (GJ feedstock/tonne H ₂) ± Uncertainty ¹	Carbon content factor 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	210 (± 20%)	0.0258	0.0238	0.0276
Plastic ³ 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%) ⁴	0.0183 ⁵	0.0148 ⁵	0.0276 ⁵

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 1.

3 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.

4 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.

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). Lower uncertainty range is from steam reforming of natural gas, upper uncertainty range is from gasification of coal.

Source:

Cormos (2011); DOE (2017); Geissler, et al. (2001); GREET (2013); Iwasaki (2003); JARI (2011); JRC (2014); Schiebahn et al. (2015); Sorensen (2011); Themelis et al. (2011); The National Energy Technology Laboratory (2017); The Pacific Northwest National Laboratory (2017); Wallman et al. (1998).

TIER 2 METHOD

In the Tier 2 methods, it is *good practice* to use country specific FRFs and/or CCFs, and to control these factors against the default factors in Table 3.30 to ensure good factor quality.

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TIER 3 METHOD

In the Tier 3 methods, it is *good practice* to use plant specific CCFs, or plant and process specific FRFs and CCFs, and to control these factors against the default factors in Table 3.30 to ensure good factor quality.

3.11.2.3 CHOICE OF ACTIVITY DATA**TIER 1 METHOD**

National or regional level activity data may be used in the Tier 1 methods. In the Tier 1a method feedstock consumption data by type of feedstock should be used, while in the Tier 1b method hydrogen production data by type of feedstock should be used. In the Tier 1c method national or regional total hydrogen production data should be used.

Double counting and gaps towards other sectors should be avoided (Box 3.16). It is *good practice* to use the Tier method giving the lowest uncertainty.

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 \pm 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.

Emissions from fuel combustion should be reported in the Hydrogen production sector only if the fuel is consumed as an integrated part of the production process, i.e. if it is taken from the feedstock. Otherwise it should be reported in the energy sector. If no information is available, it is assumed in the Tier 1 method that the fuel is taken from the feedstock.

It is *good practice* to exclude recovered (i.e. delivered to other sectors for use, or permanently stored) CO₂ from the estimated emissions, if the emissions from the downstream use are reported and/or the permanent storage is documented. If no data on recovered CO₂ could be obtained or downstream use or permanent storage cannot be documented (or properly justified), it is *good practice* to assume that the recovery is zero. See Box 3.16 for details on double counting and gaps related to recovery of CO₂.

It is *good practice* to obtain the biogenic share of the feedstock, to estimate the CO₂ emissions to be excluded from national totals and reported in a memo item. If the biogenic share cannot be obtained, it is *good practice* to assume that all feedstock is fossil.

For feedstock data obtained in tonnes, conversion can be done by using the default calorific values in Ch. 1, Vol. 1 of 2006 IPCC Guidelines.

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). Emissions from fuel combustion should be included in the Hydrogen production sector only if the fuel is consumed as an integrated part of the production process, i.e. if it is taken from the feedstock. Otherwise it should be reported in the energy sector. The biogenic share of the feedstock should be obtained from the producers, to estimate the CO₂ emissions to be excluded from national totals and reported in a memo item.

It is *good practice* to exclude recovered (i.e. delivered to other sectors for use, or permanently stored) CO₂ from the estimated emissions, if the emissions from the downstream use are reported and/or the permanent storage is documented. If no data on recovered CO₂ could be obtained or downstream use or permanent storage cannot be documented (or properly justified), it is *good practice* to assume that the recovery is zero.

Double counting and gaps towards other sectors should be avoided (Box 3.16). It is *good practice* to use the Tier method giving the lowest uncertainty.

TIER 3 METHOD

The Tier 3 methods require plant-level activity data by production method and type of feedstock. Production capacity data should not be used. Emissions from fuel combustion should be reported in the Hydrogen production sector only if the fuel is consumed as an integrated part of the production process, i.e. if it is taken from the feedstock. Otherwise it should be reported in the energy sector. The biogenic share of the feedstock should be

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obtained from the producers, to estimate the CO₂ emissions to be excluded from national totals and reported in a memo item.

If plant-level data on feedstock type and consumption cannot be provided due to confidentiality, it should be considered to distribute CCFs to the data owner, so that aggregate emission figures could be provided by the data owner instead. In such cases, the method obtains Tier 3 level if proper documentation is provided in the NIR.

It is *good practice* to exclude recovered (i.e. delivered to other sectors for use, or permanently stored) CO₂ and stored solid carbon from the estimated emissions, if the emissions from the downstream use are reported and/or the permanent storage is documented. If no data on recovered CO₂ could be obtained or downstream use or permanent storage cannot be documented (or properly justified), it is *good practice* to assume that the recovery is zero. If no information on the carbon content in the stored carbon material is available, it is *good practice* to assume that the material is pure carbon.

Double counting and gaps towards other sectors should be avoided (Box 3.16). It is *good practice* to use the Tier method giving the lowest uncertainty.

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 a and b Tiers, it is *good practice* to report as method the one giving the highest uncertainty.

To avoid double counting, emissions reported under other sectors, including Ammonia Production and Methanol Production (IPPU) and Petroleum Refining (Energy), must be excluded from hydrogen production.

Recovered CO₂ should be subtracted from hydrogen production, if emissions from its downstream use are reported and if permanent storage of recovered CO₂ is documented. If these conditions are not met (or properly justified), it is *good practice* to not subtract these recovered amounts from the CO₂ emissions.

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

3.11.2.5 DEVELOPING A CONSISTENT TIME SERIES

Recalculation of CO₂ 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 CO₂ 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 method. 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 efficient 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 c methods) have higher

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overall uncertainty than methods not using the fuel requirement factors (Tier a methods), *ceteris paribus*, because the Tier b and c methods include one uncertain element (FRF) not included in the Tier a 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 (f. ex. between different types of coal), and from variation in composition and energy content of feedstocks with a heterogeneous composition (f. ex. 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 1c 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 should be used.

If recovery occurs but the reporting of emissions from downstream use is uncertain and/or the permanent storage of recovered CO₂ is not properly documented and hence the recovery is not subtracted, a country specific uncertainty estimate or alternatively a default *increase* in the remaining uncertainty of 20 percentage points in the downward direction should be used.

3.11.3.2 ACTIVITY DATA UNCERTAINTIES

Where activity data is obtained from plants, uncertainty estimates can be obtained from the hydrogen producers. These activity data are likely to be highly accurate (i.e., with uncertainty as low as ± 2 %). This includes uncertainty estimates for feedstock use (Tier a methods) or hydrogen production (Tier b and c methods), as well as CO₂ 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 % 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 % in the uncertainty can be used for previous reference years estimates based on data on current years.

If estimating on mixed fossil and biogenic fuels in the Tier 1 and 2 methods, a default uncertainty of ± 5 % should be added to the biogenic part if it is based on reported figures, and ± 20 % if it is estimated. The same uncertainty, in absolute terms, 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 CO₂ generation rate based on natural gas should not be less than 5.46 tonnes of CO₂ per tonne of hydrogen

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produced⁶. 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.

Plant-specific data check

The following plant-specific data is 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.

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. 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.

Much of the production and process data is considered proprietary by operators, especially where there are only a small number of plants within a country. It is *good practice* to apply appropriate techniques, including aggregation of data, to ensure protection of confidential data. Guidance on managing confidential data is provided in Section 2.2, Volume 1.

⁶ Method: $44.011 \text{ tonnes CO}_2 / 8.064 \text{ tonnes H} = 5.46 \text{ tonnes of CO}_2 \text{ per tonne of H}_2 \text{ produced}$, based on molar weights of 12.011 (C), 16.00 (O), 1.008 (H) and 100% production yield (i.e. no by-products produced, no fuel combustion to produce heat and no feedstock loss in the production process).

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