

# CHAPTER 3

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## CHEMICAL INDUSTRY EMISSIONS

[Parts in yellow – comments from Authors]

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

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## 114 **3      CHEMICAL INDUSTRY EMISSIONS**

### 115 **3.1      INTRODUCTION**

116    No refinement

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118 **3.2 AMMONIA PRODUCTION**

119 No refinement

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## 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 N<sub>2</sub>O emissions.

##### TIER 2 METHOD

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

Table 3.3 includes emission factors for N<sub>2</sub>O, and associated uncertainties.

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

TABLE 3.3A DIFFERENT PLANT TYPES FOR THE PRODUCTION OF HNO <sub>3</sub> <sup>1</sup>			
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	

<sup>1</sup>InfoMil, 1999, EFMA, 2000, and Schöffel, 2001

The factors listed in Table 3.3 for plants using abatement technology, incorporate the effect of N<sub>2</sub>O 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**  
**DEFAULT FACTORS FOR NITRIC ACID PRODUCTION**

Production Process	N <sub>2</sub> O Emission Factor (relating to 100 percent pure acid)
Old (pre-1975) plants (all processes)	10-19 kg N <sub>2</sub> O/tonne nitric acid <sup>a</sup>
Single low pressure plants	5 kg N <sub>2</sub> O/tonne nitric acid ±10%
Single medium pressure plants	8 kg N <sub>2</sub> O/tonne nitric acid ±20% <sup>b</sup>
Single high pressure plants	9 kg N <sub>2</sub> O/tonne nitric acid ±40%
Single pressure plants with abatement technology*	2.5 kg N <sub>2</sub> O/tonne nitric acid ±10% <sup>c</sup>
Dual Pressure (M/H)	9 kg N <sub>2</sub> O/tonne nitric acid ±30% <sup>d</sup>
Dual Pressure (M/H) with abatement technology	2.5 kg N <sub>2</sub> O/tonne nitric acid ±20% <sup>d</sup>
Dual Pressure (L/M)	7 kg N <sub>2</sub> O/tonne nitric acid ±10% <sup>d</sup>
Dual Pressure (L/M) with abatement technology	1.5 kg N <sub>2</sub> O/tonne nitric acid ±10% <sup>d</sup>
<p>Notes:</p> <p>*All single pressure plants using N<sub>2</sub>O abatement measures such as process-integrated or tailgas N<sub>2</sub>O destruction or non-selective catalytic reduction (NSCR, a NO<sub>x</sub> abatement technology that can also be managed to abate N<sub>2</sub>O).</p> <p>Sources:</p> <p><sup>a</sup> Based on IPCC 2000 Good Practice Guidance and Uncertainty Management in National Greenhouse Gas Inventories and the tests from CDM projects presented in USEPA 2010 Available and Emerging Technologies for Reducing Greenhouse Gas Emissions from the Nitric Acid Production Industry, December 2010.</p> <p><sup>b</sup> Based on 2017 Annex I Party GHG Inventory Submissions available at <a href="http://unfccc.int/national_reports/annex_i_ghg_inventories/national_inventories_submissions/items/10116.php">http://unfccc.int/national_reports/annex_i_ghg_inventories/national_inventories_submissions/items/10116.php</a> and Joint Implementation projects (8 track 1 and 3 track 2) available at <a href="http://ji.unfccc.int/JI_Projects/ProjectInfo.html">http://ji.unfccc.int/JI_Projects/ProjectInfo.html</a>.</p> <p><sup>c</sup> Inclusion of all abatement technologies in a single category using the values from IPCC 2006, "Guidelines for National Greenhouse Gas Inventories, Volume 3 Industrial Process and Product Use, Chapter 3 Chemical Industry Emissions" and applying a conservativeness factor for NSCR.</p> <p><sup>d</sup> Based on information from European industrial plants published in European Commission (EC), 2007, "Reference Document on BAT (Best Available Techniques) for the Manufacture of Large Volume Inorganic Chemicals (Ammonia, Acids and Fertilizers)", August 2007 and European Commission (EC), 2009, Ecofys, Fraunhofer Institute for Systems and Innovation Research, and Öko-Institut, 2009, Methodology for the free allocation of emission allowances in the EU ETS post 2012 Sector report for the chemical industry, The European Commission, November 2009, 2017 Annex I Party GHG Inventory Submissions available at <a href="http://unfccc.int/national_reports/annex_i_ghg_inventories/national_inventories_submissions/items/10116.php">http://unfccc.int/national_reports/annex_i_ghg_inventories/national_inventories_submissions/items/10116.php</a> and Joint Implementation projects (8 track 1 projects and 3 track 2 projects) available at <a href="http://ji.unfccc.int/JI_Projects/ProjectInfo.html">http://ji.unfccc.int/JI_Projects/ProjectInfo.html</a>.</p>	

### TIER 3 METHOD

Plant measurements provide the most rigorous data for calculating net emissions (i.e., N<sub>2</sub>O generation and destruction factors). Monitoring N<sub>2</sub>O emissions from nitric acid production is practical because these are point sources and there are a finite number of production plants. Given currently available technology, instrumentation for sampling and monitoring emission rates do not limit precision or accuracy of the overall measurement. Usually sampling frequency and timing is sufficient to avoid systematic errors and to achieve the desired level of accuracy.

As a general rule, it is *good practice* to conduct sampling and analysis whenever a plant makes any significant process changes that would affect the generation rate of N<sub>2</sub>O, 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



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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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183 **3.4 ADIPIC ACID PRODUCTION**

184 No refinement

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186 **3.5 CAPROLACTAM, GLYOXAL AND GLYOXYLIC**  
187 **ACID PRODUCTION**

188 No refinement

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190 **3.6 CARBIDE PRODUCTION**

191 No refinement

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193 **3.7 TITANIUM DIOXIDE PRODUCTION**

194 No refinement

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196 **3.8 SODA ASH PRODUCTION**

197 No refinement

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199 **3.9 PETROCHEMICAL AND CARBON BLACK**  
200 **PRODUCTION**

201 No refinement

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

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

Where:

 $E_{HFC-23}$  = by-product HFC-23 emissions from HCFC-22 production, kg $EF_{default}$  = HFC-23 default emission factor, kg HFC-23/kg HCFC-22 $P_{HCFC-22}$  = total HCFC-22 production, kg

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

**Tier 2**

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

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

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

Where:

 $E_{HFC-23}$  = by-product HFC-23 emissions from HCFC-22 production, kg $EF_{calculated}$  = HFC-23 calculated emission factor, kg HFC-23/kg HCFC-22 $P_{HCFC-22}$  = total HCFC-22 production, kg $F_{released}$  = Fraction of the year that this stream was released to atmosphere untreated, fraction

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

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

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

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

Where:

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

CBE = carbon balance efficiency, percent

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

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

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**EQUATION 3.33****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****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 3.35A****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:

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

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

Where:

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

**Tier 3a**

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

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

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

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

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

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'

$F_i$  = 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****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 m<sup>3</sup>/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****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

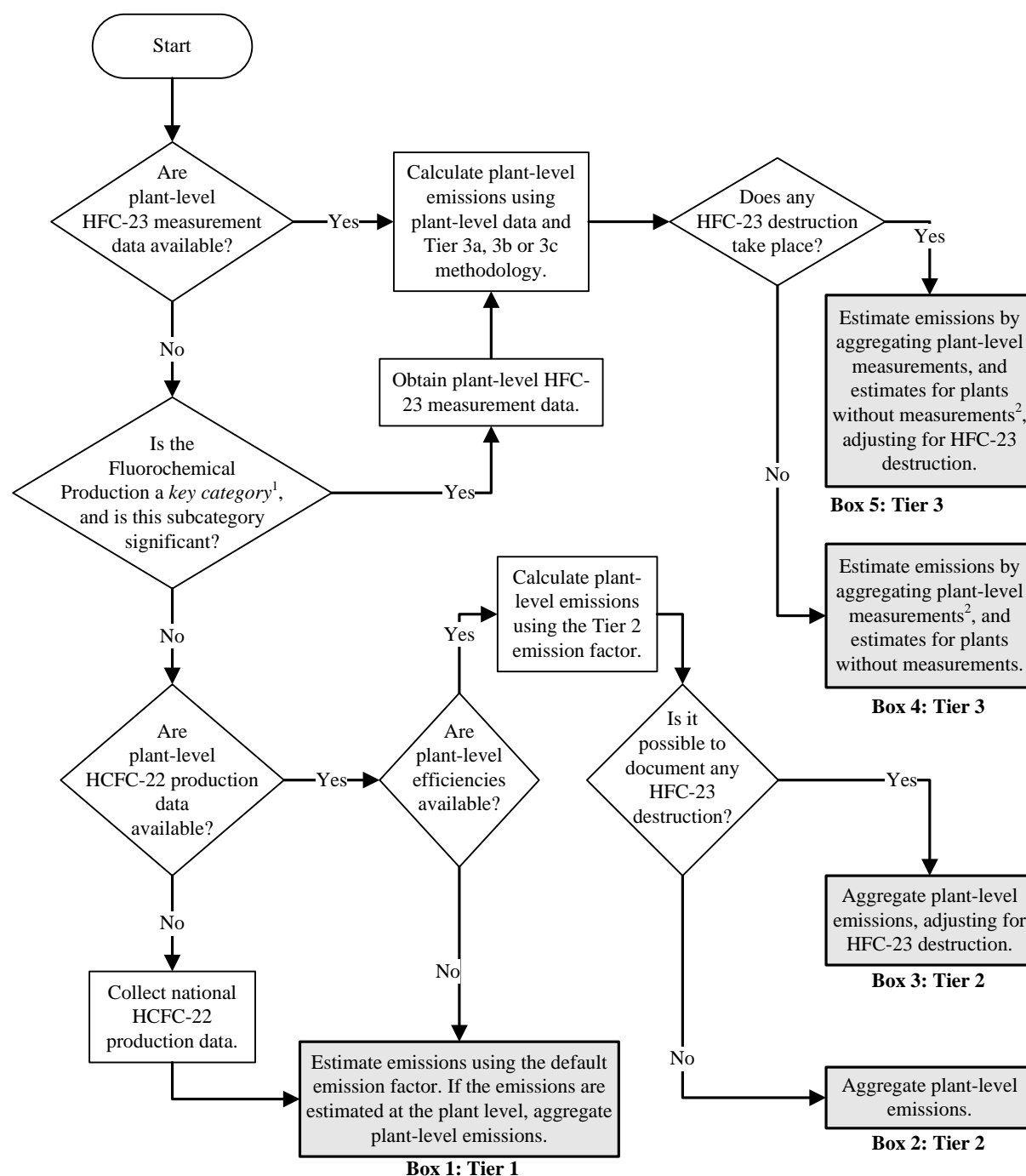
Material recovered for uses where it may be emitted potentially may be counted here if the emissions are included in the quantity calculated by the methods in Chapter 7 of this volume.

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.

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



Note:

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

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

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

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**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**  
**HFC-23 DEFAULT EMISSION FACTORS**

<b>Technology</b>	<b>Emission Factor (kg HFC-23/kg HCFC-22 produced)</b>
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) <sup>1</sup>	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>

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

**Box 3.14****PLANT MEASUREMENT FREQUENCY**

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

(RTI, Cadmus, 1998)

**CHOICE OF ACTIVITY DATA**

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

**COMPLETENESS**

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

**DEVELOPING A CONSISTENT TIME SERIES**

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

**3.10.1.3 UNCERTAINTY ASSESSMENT**

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 SF<sub>6</sub>, CF<sub>4</sub>, C<sub>2</sub>F<sub>6</sub>, C<sub>3</sub>F<sub>8</sub>, C<sub>4</sub>F<sub>10</sub>, C<sub>5</sub>F<sub>12</sub> and C<sub>6</sub>F<sub>14</sub> were reported (UNFCCC, 2005). Other examples include the release of by-product N<sub>2</sub>O and CF<sub>4</sub> from the production of NF<sub>3</sub> (Tasaka, 2004; 2007), CF<sub>4</sub> from the production of CFC-11 and 12, or of SF<sub>6</sub> from the production of uranium hexafluoride in the nuclear fuel cycle.

Typically, fluorochemicals may be released from chemical processes involving a broad range of technologies and processes<sup>2</sup>:

- Telomerization Process used in the production of fluorochemicals fluids and polymers
- Photooxidation of tetrafluoroethylene to make fluorochemical fluids
- Direct Fluorination often used in SF<sub>6</sub> production
- Halogen Exchange Processes to make low boiling PFCs like C<sub>2</sub>F<sub>6</sub> and CF<sub>4</sub>, HFC 134a and 245fa
- NF<sub>3</sub> manufacturing by direct fluorination
- Production of uranium hexafluoride
- Production of fluorinated monomers like tetrafluoroethylene and hexafluoropropylene
- Production of fluorochemical agrochemicals

<sup>2</sup> 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 SF<sub>6</sub> require elemental fluorine, generated electrochemically. In 'electrochemical fluorination' processes, the fluorine is not separated but makes the desired product in the electrochemical cell. In other processes it is separated and subsequently used, either as the elemental gas or as a component of a carrier system, such as CoF<sub>3</sub>. 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. The Tier 1 default emission factor is intended to cover emissions for both process vents and equipment leaks. 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 may be evacuated from the container, and these are also an emission source.

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. The number of major producers of these fluorinated greenhouse gases is quite small: in the case of SF<sub>6</sub>, there are globally about **X** companies with about **X** production facilities world-wide. A survey of national producers should not be difficult to compile.

[ *Authors continue to search alternative sources to find how many factories exist worldwide* ]

#### Tier 1

In the Tier 1 methodology, a default emission factor, or a similar number derived for the particular country's circumstances, can be used to estimate national production-related emissions of individual HFCs, PFCs, SF<sub>6</sub> and other fluorinated greenhouse gases. The default emission factors in Table 3.29 are expressed in terms of kg CO<sub>2</sub>e emitted/kg CO<sub>2</sub>e produced (that is, both emissions and production are GWP-weighted). [We are considering presenting default emission factors in terms of kg CO<sub>2</sub>e emitted/kg fluorinated compound produced, which would better account for the fact that high-GWP emissions may result from the production of low-GWP products.]

#### EQUATION 3.41 TIER 1 CALCULATION OF PRODUCTION-RELATED EMISSIONS

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

Where:

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

$EF_{\text{default}, k}$  = 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 SF<sub>6</sub> 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 quantity of emissions estimated from the difference in the sum of masses of reactants and products and 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* (in which case, Tier 3 methodology is specified). As described in Equation 3.41A, should the chemical composition of the mass of material emitted from the process be determined through chemical analysis, the Tier 2 estimate is further improved:

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

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

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 the process, kg/kg

$M_{ijk}$  = mass emitted from  $j$  streams in each plant over all  $i$ , plants 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

**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 3.42A where emissions are summed over all streams  $j$ , all equipment types  $g$ , at all plants  $i$ , over a given time period  $t$ .

**EQUATION 3.42A****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  $k$ .

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

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$E_{kEL}$  = 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 3.42B****TIER 3 DIRECT CALCULATION OF PRODUCTION-RELATED EMISSIONS FROM PROCESS VENTS**

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

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 3.43A****TIER 3 CALCULATION OF PRODUCTION-RELATED EMISSIONS FROM PROCESS VENTS USING A SITE- OR PROCESS-SPECIFIC EMISSION FACTOR**

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

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.

**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 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).

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**EQUATION 3.43B**  
**TIER 3 CALCULATION OF EMISSIONS FROM EQUIPMENT LEAKS USING A SCREENING RANGES**  
**APPROACH**

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

$E_{gijkEL}$  = 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  $i$ .

$C_{ijk}$  = 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 3.43C**  
**TIER 3 CALCULATION OF EMISSIONS FROM EQUIPMENT LEAKS USING A CORRELATION**  
**APPROACH**

$$E_{gijkEL} = \left( Slope_g \times (SV_{jgk})^{CE_g} \right) \times C_{ijk}$$

$E_{gijkEL}$  = 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  $g$ .

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

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

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

The third approach for estimating equipment leak emissions is the Unit-Specific Correlation approach. In the Unit-Specific Correlation approach, selected mass emission rates are determined by an equipment bagging procedure, and the associated screening value (concentration) is concurrently measured. This set of data is used to develop a unit-specific correlation 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 3.43D.

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**EQUATION 3.43D**  
**TIER 3 CALCULATION OF A UNIT-SPECIFIC CORRELATION**

$$\log_{10} E_{ijkEL} = (\beta_0 + \beta_1 \times SV_{ijgk})$$

Where

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

$\beta_0$  = intercept of regression equation.

$\beta_1$  = slope of regression equation.

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

**EQUATION 3.43E**  
**TIER 3 CALCULATION OF EMISSIONS FROM EQUIPMENT LEAKS USING A UNIT-SPECIFIC CORRELATION APPROACH**

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

$E_{ijkEL}$  = 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 3.43F where emissions are summed over all streams  $j$ , equipment types  $g$ , at all plants  $i$ , over a given time period  $t$ .

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

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

Where:

$E_{kEL}$  = total equipment leak, production-related emissions of fluorinated greenhouse gas  $k$ :  $E_{ijkEL}$  = 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 3.43B, 3.43C, or 3.43E.

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

## CHOICE OF EMISSION FACTORS

### Process Equipment

Tier 3 relies on direct measurements of, or the use of, process and facility specific emission factors to determine the quantities of individual materials 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 the fluorinated greenhouse gas. For Tier 1, the default emission factors in Table 3.29 assume there is no use of abatement, and these default emission factors

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include emissions from both process vents and equipment leaks (U.S. EPA, 2017a, U.S. EPA, 2017b). There is a wide range of substances that may potentially be released. Some data show that the components that are lost during production of a particular fluorochemical have, in general, radiative forcing properties similar to those of the desired fluorochemical (AFEAS 2004). Consequently, for sources that are not significant subcategories under *key category*, product, reactant, and by-product emissions may be assumed to consist of the same gases, however this relationship does not hold for all production processes.

## Tier 1 Default Emission Factors

TABLE 3.29A DRAFT FLUORINATED GHG DEFAULT EMISSION FACTORS	
F GHG emission factor for process vents and equipment leaks	Emission Factor (kg CO <sub>2</sub> e/kg HFC or Fully F CO <sub>2</sub> e produced)
Emission factor for HFCs	[0.05 to 0.1]
Uncertainty for emission factor for HFCs	[To be determined]
Emission factor for fully fluorinated compounds	[To be determined from U.S. EPA 2017a and 2017b]
Uncertainty for emission factor for fully fluorinated compounds	[To be determined]
<sup>a</sup> Data from the U.S. GHGRP are currently publicly available for certain fluorinated GHG Groups, for example, HFCs. Data for fully fluorinated compounds (fully F) may also be released in the future, in which case emission factor values will be provided when the data are released.	

The default emission factors listed in Table 3.29 were estimated using data from U.S. EPA 2017a and 2017b, described in detail by Schaffner (2017). Under the Greenhouse Gas Reporting Program, fluorinated GHG emissions are reported on a facility basis and include facilities with and without abatement. To develop emission factors on an uncontrolled basis, the pre-abatement emissions were estimated using the arithmetic average of facility-reported DE ranges, and the default emission factor was calculated by normalizing the estimated, pre-abatement fluorinated GHG emissions by the net supply of fluorinated GHG. As HFCs and PFCs can be emitted from fluorinated GHG manufacturing processes other than those producing HFC and PFCs, the uncertainty and details of the calculations used to calculate the default EFs are discussed in Schaffner, 2017.

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. In the case of SF<sub>6</sub>, based on German experience, a default emission factor of 0.002 of the total quantity of SF<sub>6</sub> produced is suggested for those countries in which the predominant end use does not require highly purified SF<sub>6</sub> gas (e.g., electrical equipment, insulated windows) (Preisegger, 1999). [Note: It is not known whether the 0.002 factor is based on pre-abatement emissions or controlled, post-abatement emissions.] Based on experience in Japan, in countries where the major uses require highly purified SF<sub>6</sub> gas (e.g., semiconductor manufacturing), the default value should be 0.08 because of handling losses during disposal of residual gas (i.e., the 'heel' that is not used or recycled) in returned cylinders (Suizu, 1999). A low and realistic SF<sub>6</sub> emission factor has been reported as 0.03 of sales (O'Connell 2002). U.S. and Japanese NF<sub>3</sub> manufacturers have reported an emission factor 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). CF<sub>4</sub> and N<sub>2</sub>O are generated as a by-product during NF<sub>3</sub> manufacture, N<sub>2</sub>O and CF<sub>4</sub> can be formed at rates of 0.03 and less than 0.01, respectively, relative to the mass of NF<sub>3</sub> 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 EF 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 factors in Table 3.29.

**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

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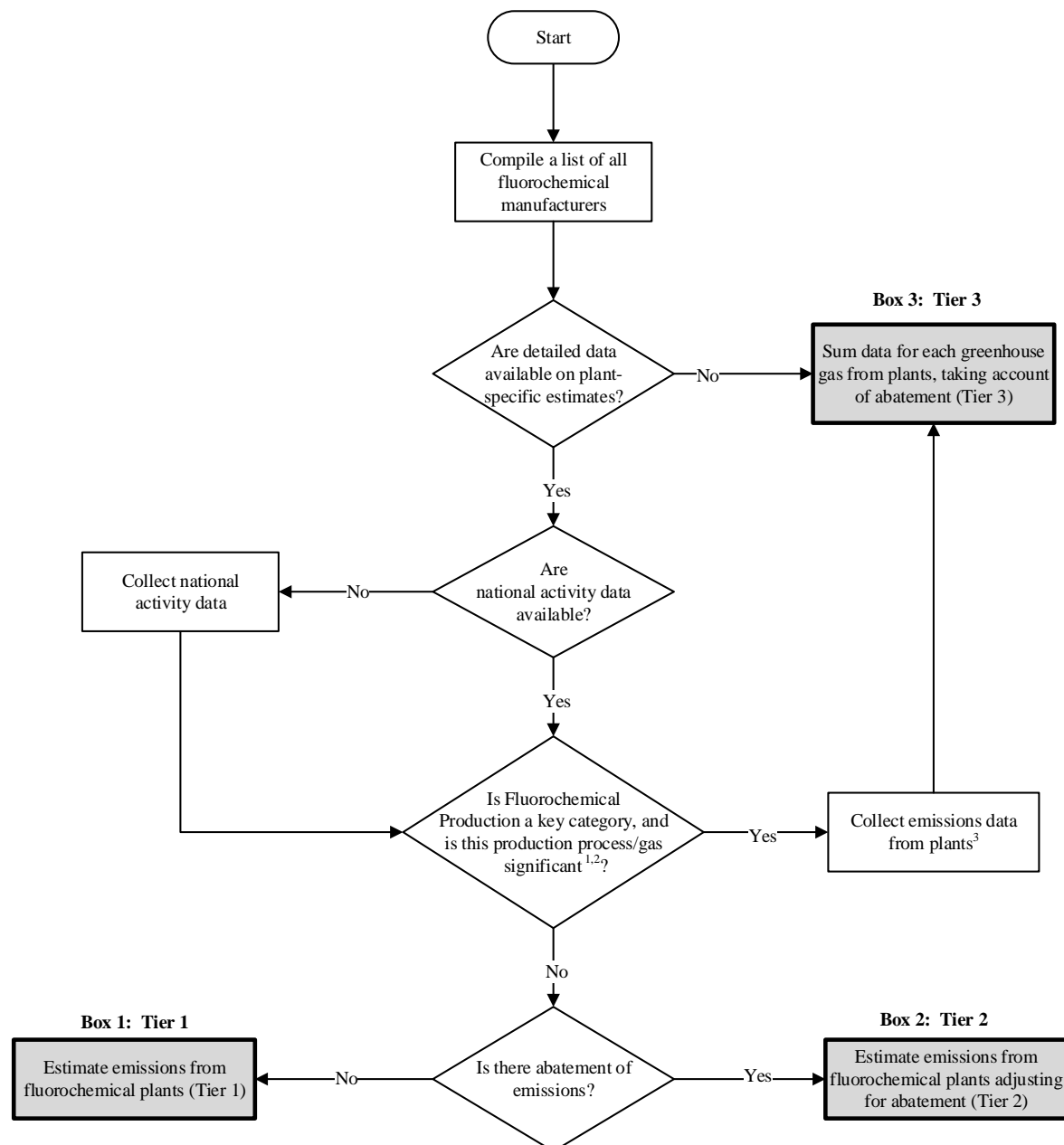
efficiency of 100 percent is suggested. As an example, when a thermal oxidation unit is well-operated and well-maintained, it has been shown to reduce HFC-23 emission by 99.996 percent (Irving, 2000). However, the on-line time of the destruction process can also have a significant effect on emissions and should be recorded. For example, in the case of a treatment system with 99 percent removal efficiency, the magnitude of fluorinated GHG emissions would be dominated by the amount of process uptime.

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



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**Figure 3.17** Decision tree for emissions of fluorinated greenhouse gases from production processes, applicable to both fugitive and by-product emissions [decision tree may be refined further]



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. Tier 2 methodology may be used at this point to establish whether or not this is a key category but, as explained in Section 3.10.2.2, this is the only use for Tier 2.

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

## 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.

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**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 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. In supporting background data for the default emission factors, the estimated destruction efficiency data were reported as a range for each process, and the assumptions related to destruction efficiency affect the uncontrolled, pre-abatement emission estimates used in the factors. Because there are numerous processes and therefore numerous data points in the background data, the uncertainty related to the destruction efficiency estimated for each individual process tends to balance out and the aggregate uncertainty is reduced. (Note: Based on assumptions regarding the DE used to calculate the pre-abatement emissions from the data reported to U.S. EPA (2017a), the default EF can range from 1 to 20 percent, falling within the uncertainty listed in the 2006 version of the guidelines.) In addition, the default emission factor analysis assumes that the characteristics of fluorinated GHG emitted from the process are similar to those of the product, however this is not true for all processes. For example, we assumed that HFCs are emitted from the production of HFC products, however HFCs may also be released from the production of other types of products, therefore the emission factor is for HFCs may be overestimated.

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

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

No Refinement

## 3.11 HYDROGEN PRODUCTION

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*.

### 3.11.1 Introduction

The dominating hydrogen production technologies are steam reforming and gasification (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, a series of enhancement and purification steps yields a highly pure hydrogen output (99.999% purity is normal at present). Other production methods are biological technologies, like fermentation and photo biological water splitting, electrolytic technologies, photo catalytic technologies and thermolysis. Steam reforming and gasification produce CO<sub>2</sub> and very minor amounts of methane. Biological technologies produce no fossil CO<sub>2</sub>, but might generate minor amounts of methane; at present a maximum of 2% is normal (Braga et al 2017). However, these methods produce hydrogen in a very small scale at present. Other technologies produce no CO<sub>2</sub> from the production process itself, but methods like reforming of ammonia and thermolysis require high temperatures and might involve combustion of fossil fuels.

Only production methods generating greenhouse gases from fossil feedstocks should be included in GHG totals in the inventory. Emissions of CO<sub>2</sub> from thermochemical processes like fuel reforming and gasification using biomass as feedstock should be accounted for in the IPPU memo item. Emissions of GHG from biological processes are considered negligible and should not be reported. Production methods generating no direct greenhouse gas emissions, like electrolysis of water, should not be considered in IPPU GHG totals.

Hydrogen is produced as a main product, a by-product for sale, or as an intermediate product in f. ex. refineries or ammonia factories for use in later production steps. Only emissions from production of hydrogen as the main product should be reported in this sector. When hydrogen is produced as a by-product or intermediate product, it is good practice to report the CO<sub>2</sub> emissions in the sector of the main product, Table 3.29. For instance, intermediate hydrogen production in refineries or ammonia plants is covered in the respective sectors (i.e. refineries or ammonia production). See Box 3.18 for details about double counting. If hydrogen is produced in situ, for instance in a vehicle in combination with a fuel cell, the emissions should be reported in the sector of the consumer.

The most common production methods at present, accounting for more than 95 per cent of the global hydrogen production, are reforming and gasification of fossil fuels with water gas shift reaction. Several types of fossil fuels, like natural gas, naphtha, coal and lignite, are used as feedstock. The remaining production is mainly done by electrolysis. 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).

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

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TABLE 3.29 CURRENT HYDROGEN PRODUCTION METHODS – STATUS OF DEVELOPMENT AND ALLOCATION OF EMISSIONS TO SECTOR				
Category	Technology	Feedstock	Status of development	Sector
Main product hydrogen	Fuel reforming	Fossil	Major technology	Hydrogen
		Biofuel	Minor and increasing	Memo IPPU
		Waste	Minor and increasing	Hydrogen/Memo IPPU
		Ammonia	Minor and increasing	Energy (stationary combustion) <sup>1</sup>
		Methanol <sup>2</sup>	Experimental	Sector of consumer
	Gasification	Fossil	Major technology	Hydrogen
		Biomass	Minor and increasing	Memo IPPU
		Waste	Minor and increasing	Hydrogen/Memo IPPU
	Water electrolysis	Water	Minor and mature	No emissions
	Fermentation	Biomass	Experimental	Insignificant emissions
	Photo voltaic	Water	Experimental	No emissions
	Thermal water splitting	Water	Experimental	Energy (stationary combustion)
	Photo catalytic splitting	Water	Experimental	No emissions
	Photo biological splitting	Water	Experimental	No emissions
By-product or intermediate product hydrogen	Refineries	All	Major technology	Energy (stationary combustion)
	Ammonia production	All	Major technology	Ammonia production
	Methanol production	All	Major technology	Petrochemical industries
	Ethylene production	All	Minor technology	Petrochemical industries
	Steel production	All	Minor technology	Steel production
	Soda production	Soda	Minor technology	No emissions

<sup>1</sup> The emissions arise from combustion of fuels to power the reforming reaction.<sup>2</sup> Reforming of methanol is mainly a technology developed for in situ use, in combination with fuel cell systems.

### BOX 3.15 USES OF HYDROGEN

Hydrogen (H<sub>2</sub>) 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.

The estimation methods described in this section have hydrogen *production* as their starting point. Therefore, the emission estimates are independent of how hydrogen is being used.

## 3.11.2 Methodological issues

The most widespread methods for hydrogen production at present are, by far, steam reforming and gasification (i.e. oxidation) of fossil feedstocks. Oxidation of fossil feedstocks generates CO<sub>2</sub>, and efforts are made to develop alternative methods with no (or reduced) GHG emissions. However, other methods are used as well. At present,

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most of these methods are at an experimental level, while some are commercially available (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. Complete oxidation technologies have hydrogen as the main product, and the CO<sub>2</sub> emissions can be estimated with low uncertainty from feedstock consumption data. Partial oxidation technologies have hydrogen as a by-product or intermediate product.

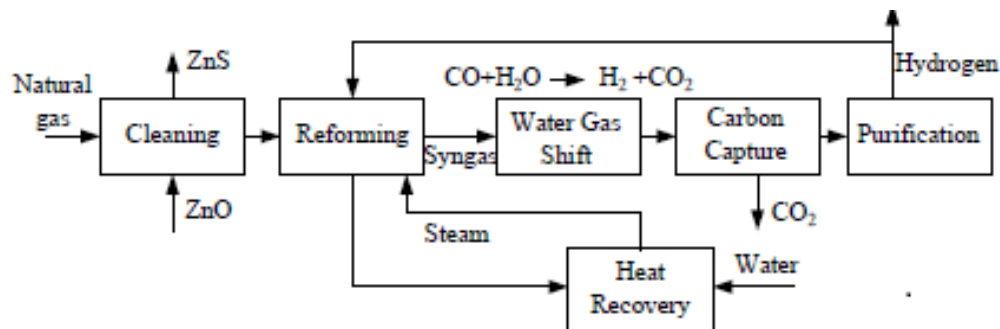
## COMPLETE OXIDATION TECHNOLOGIES

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). The production process has several steps. 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. Both steps are endothermic. A final combustion reaction completes the oxidation of the carbon and produces energy that fuels the production process.

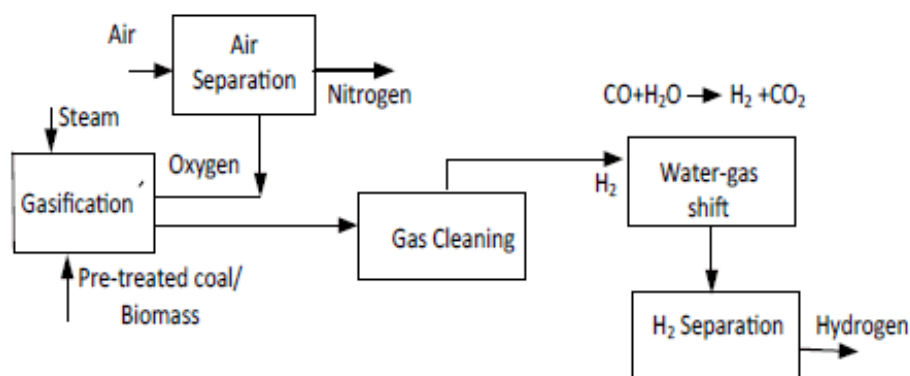
In both the hydrogen producing steps (overall reaction) and the combustion there is an approximate 1:1 molar relation between the produced CO<sub>2</sub> and the carbon contained in the feedstock. The only exceptions are solid carbon residues disposed of as waste.

Other feedstocks are sometimes used as well, though in a very small scale at present. If the feedstock is biogenic, the CO<sub>2</sub> should be placed in the IPPU memo item. Waste may contain both fossil and biogenic materials. The same applies to fossil fuels with biofuel mixed in. The CO<sub>2</sub> emissions from feedstocks containing a mix of fossil and biogenic carbon should be allocated partly to the hydrogen sector and partly to the IPPU memo item, relative to the respective fossil and biogenic carbon shares.

**Figure 3.18 Hydrogen production via steam reforming with water gas shift reaction**



**Figure 3.19 Hydrogen production via gasification with water gas shift reaction<sup>1</sup>**



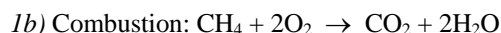
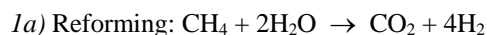
<sup>1</sup> The flue gas from the H<sub>2</sub> separation step, containing CO and methane, is burnt in a boiler to produce heat (i.e. steam).

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

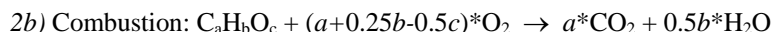
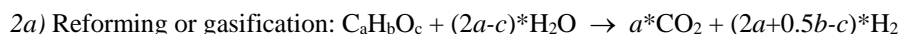
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**Box 3.16****CHEMICAL REACTIONS IN HYDROGEN PRODUCTION BY COMPLETE OXIDATION TECHNOLOGIES**

Steam reforming of natural gas (overall reactions):

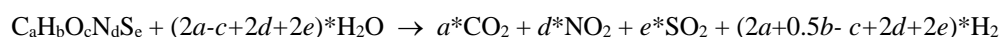


Steam reforming or gasification of other fossil or biogenic feedstocks (overall general formulas):

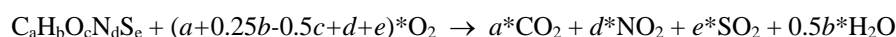


Gasification of waste (overall general formulas):

3a) Gasification:



3b) Combustion:



In all these overall reactions the ratio of consumed feedstock carbon to produced  $\text{CO}_2$  molecule is 1:1. The molar relation between each reforming/gasification reaction and the subsequent combustion reaction depends on the efficiency of the production process, and the ratio of produced hydrogen to produced  $\text{CO}_2$  varies accordingly. (Trane et al. 2012,... [applies to steam reforming of biogenic feedstocks; more literature sources will be added])

**PARTIAL OXIDATION TECHNOLOGIES**

Partial oxidation technologies (incl. autothermal reforming) are reforming and gasification technologies consisting of the first reaction steps in a complete oxidation production method, but without all the subsequent steps (f. ex. water gas shift reaction) that complete the carbon oxidation. Production of hydrogen by partial oxidation technologies mainly uses coal or natural gas as input. The output from the reaction is syngas (see Box 3.17 for details about syngas), which in most cases is the final product. In other cases, the syngas is separated into its component gases in a second step. In both cases the GHGs are part of the produced gas and should not be reported as an emission in the hydrogen sector (Table 3.29).

**Box 3.17****SYNGAS**

Syngas is a mixture of carbon monoxide, hydrogen and other gases. Syngas is produced by partial oxidation or autothermal reforming of natural gas, coal or other carbon containing fuels. It is primarily produced as an intermediate in refineries and in manufacturing of chemicals, but production as an energy product or as a by-product for commercial sale, either as a mixture or separated into its single gases, also occurs.

The  $\text{CO}_2$  and methane are parts of the syngas, and hence parts of the product. Therefore, the GHGs from syngas production should not be reported. The GHG emissions from use of syngas should be reported in the sector where it is used.

**OTHER PRODUCTION METHODS**

Production by water electrolysis is widespread but mainly in small-scale plants, and accounts for about 4 per cent of current hydrogen production. Other methods for hydrogen production are currently at a minor or experimental level. Several of the methods, f. ex. water electrolysis and photo induced water splitting, are without direct GHG



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emissions. Others, f. ex. fuel reforming of ammonia and thermal water splitting, have all their emissions arising from stationary combustion of fuels, and accordingly the emissions are allocated to the energy sector.

Biological methods like 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 CO<sub>2</sub>, methane and other organic substances, and CO<sub>2</sub> off-gas. Biological methods are still in a very small-scale use, and moreover parts of the CO<sub>2</sub> are captured by the microbes. Hence, the emitted CO<sub>2</sub> is considered negligible. Methane emissions make up a maximum of 2% of the hydrogen production, and are considered insignificant as well.

This means, in effect, that no production methods other than steam reforming and coal gasification should be considered 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 1 and 2 methods are based on hydrogen production data, only, while on Tier 3 level there are methods based on both hydrogen production data and feedstock (i.e. raw material and fuel) data. Note that *only the part of hydrogen production having hydrogen as its main product (i.e. not intermediate product or by-product) should be included*, to avoid double-counting with other sectors, Box 3.18.

If all relevant activity data is available, it is *good practice* to choose the method having the lowest overall uncertainty. A higher Tier method has a lower uncertainty, and the Tier 3b method has a lower uncertainty than the Tier 3a method.

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

#### TIER 1 METHOD

The Tier 1 method uses total national amounts of hydrogen produced together with data on recovered CO<sub>2</sub> to derive emissions, and should be used if more detailed data on feedstock consumption or hydrogen production is not available and hydrogen production is not a *key category*. If data on total national hydrogen production is not available, it is *good practice* to use hydrogen production capacity data instead. [Using capacity data as activity data is offered in the ammonia chapter. Hence, it is considered to be an appropriate option here as well (though not the preferred option).]

The CO<sub>2</sub> emissions are estimated as follows:

$$\text{E}_{\text{CO}_2} = \sum (\text{HP} \bullet \text{FRF} \bullet \text{CCF} \bullet 44/12) - \text{R}_{\text{CO}_2}$$

Where:

$\text{E}_{\text{CO}_2}$  = emissions of CO<sub>2</sub> (tonnes)

HP = 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)

$\text{R}_{\text{CO}_2}$  = CO<sub>2</sub> recovered (tonnes)

Aggregate hydrogen production data (HP) from national statistics may be used in the Tier 1 method. If adequate production data is not available, production capacity data may be used instead. It is *good practice* to avoid double counting with other sectors (Box 3.18). The feedstock requirement factor (FRF) converts the production of hydrogen into the corresponding consumption of feedstock (i.e. raw material and fuel). The default value is given in Table 3.30. The carbon content factor (CCF) converts the feedstock into carbon equivalents, while 44/12 converts the carbon into CO<sub>2</sub> (see Section 3.11.2.2 for details). The default carbon content factor is given in Table 1.3 in Vol.2, Chapter 1 of the IPCC 2006 Guidelines.

[CCF for plastic is missing in Vol.2 Chapter.1, but is needed for hydrogen production. CCF<sub>plastic</sub> = 20.0 kg/GJ (uncertainty not assessed yet). Wallman et al.: HYDROGEN PRODUCTION FROM WASTES, Energy Vol. 23, No. 4, pp. 271–278, 1998. Moreover, a default CCF<sub>total</sub> is estimated as: CCF<sub>total</sub> = 18.3 kg/GJ (lower = 14.8,

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upper = 27.6). Average based on CCFs from Vol.2 Chapter.1 and weighted according to global hydrogen production by feedstock type].

It is assumed that the same type of material is used for both raw material and fuel in a given production method. If different materials are being used for raw material and fuel, it is *good practice* to use the CCF for the raw material. Emissions reported in other sectors should be excluded to avoid double counting (Box 3.18). If the production data cannot be split by type of feedstock, it is *good practice* to use the general default CCF value from table 3.11.2.

If the feedstock contains biogenic components (f. ex. biodiesel, waste, etc.), the CO<sub>2</sub> emission (E<sub>CO2</sub>) should be allocated partly to the hydrogen sector and partly to the IPPU memo item, relative to the respective fossil and biogenic carbon shares. If the biogenic share cannot be estimated, it is *good practice* to assume that all feedstock is fossil.

Recovered CO<sub>2</sub> is typically sold for use in other manufacturing industries, but could also be sent to permanent storages. It is *good practice* to exclude recovered CO<sub>2</sub> from the estimated emissions. If no data on recovered CO<sub>2</sub> could be obtained, it is *good practice* to assume that the recovery is zero. CO<sub>2</sub> recovered for use in other manufacturing industries, for example industrial CO<sub>2</sub> 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 include these emissions in the respective sectors.

## TIER 2 METHOD

The Tier 2 method uses aggregate hydrogen production data together with data on recovered CO<sub>2</sub> to derive emissions, and should be used when plant-specific data on feedstock consumption or hydrogen production is not available. The production data used in the Tier 2 method should be split according to type of feedstock being used. The CO<sub>2</sub> emissions are estimated as follows:

$$\text{E}_{\text{CO}_2} = \sum_j (\text{HP}_j \cdot \text{FRF}_j \cdot \text{CCF}_j \cdot 44/12) - \text{R}_{\text{CO}_2}$$

Where:

E<sub>CO2</sub> = emissions of CO<sub>2</sub> (tonnes)

HP<sub>j</sub> = hydrogen produced as main product, feedstock *j* (tonnes)

FRF<sub>j</sub> = feedstock requirement per unit of output, feedstock *j* (GJ feedstock / tonne hydrogen produced)

CCF<sub>j</sub> = carbon content factor, feedstock *j* (tonne C / GJ feedstock)

R<sub>CO2</sub> = CO<sub>2</sub> recovered (tonnes)

Aggregate hydrogen production data (HP<sub>j</sub>) from national statistics may be used in the Tier 2 method. It is *good practice* to avoid double counting with other sectors (Box 3.18). Default feedstock specific feedstock requirement factors (FRF<sub>j</sub>) and carbon content factors (CCF<sub>j</sub>) are given in Table 1.3 in Vol.2, Chapter.1. If hydrogen production is not a *key category*, up to 5% [this percentage might be replaced with a default estimated percentage, based on the factor uncertainties] of national total hydrogen production volume may have unknown type of feedstock in the estimations. In this case, it is *good practice* to use the default general FRF and CCF.

The feedstock requirement factor converts the production of hydrogen into the corresponding consumption of feedstock (i.e. raw material and fuel). The carbon content factor converts the feedstock into carbon equivalents, while 44/12 converts the carbon into CO<sub>2</sub> (see Section 3.11.2.2 for details). It is assumed that the same type of material is used for both raw material and fuel in a given production method. If different materials are being used for raw material and fuel, it is *good practice* to use the CCF for the raw material. Emissions reported in other sectors should be excluded to avoid double counting (Box 3.18). If an adequate split of the production data by type of feedstock is unavailable, it is *good practice* to use the Tier 1 method.

If the feedstock contains biogenic components (f. ex. biodiesel, waste, etc.), the CO<sub>2</sub> emission (E<sub>CO2</sub>) should be allocated partly to the hydrogen sector and partly to the IPPU memo item, relative to the respective fossil and biogenic carbon shares. If the biogenic share cannot be estimated, it is *good practice* to assume that all feedstock is fossil.

Recovered CO<sub>2</sub> is typically sold for use in other manufacturing industries, but could also be sent to permanent storages. It is *good practice* to exclude recovered CO<sub>2</sub> from the estimated emissions. CO<sub>2</sub> recovered for use in other manufacturing industries, for example industrial CO<sub>2</sub> used in freezing applications, will most often be emitted



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to the atmosphere in the respective manufacturing industry or during use of the manufactured product. It is *good practice* to include these emissions in the respective sectors.

### TIER 3A METHOD

The Tier 3a method uses the amount of hydrogen produced on a plant-level together with data on recovered CO<sub>2</sub> and stored amounts of carbon to derive emissions. The CO<sub>2</sub> emissions are estimated as follows:

$$E_{\text{CO}_2} = \sum_{i,j,n} (\text{HP}_{i,j,n} \bullet \text{FRF}_{i,j,n} \bullet \text{CCF}_j \bullet 44/12) - (\text{R}_{\text{CO}_2} + \text{S}_C \bullet 44/12)$$

Where:

$E_{\text{CO}_2}$  = emissions of CO<sub>2</sub> (tonnes)

$\text{HP}_{i,j,n}$  = hydrogen produced as main product, process  $i$  and feedstock  $j$  and plant  $n$  (tonnes)

$\text{FRF}_{i,j,n}$  = feedstock requirement per unit of output, process  $i$  and feedstock  $j$  and plant  $n$  (GJ feedstock / tonne hydrogen produced)

$\text{CCF}_j$  = carbon content factor, feedstock  $j$  (tonne C / GJ feedstock)

$\text{R}_{\text{CO}_2}$  = CO<sub>2</sub> recovered (tonnes)

$\text{S}_C$  = carbon stored (tonnes)

Plant specific hydrogen production data ( $\text{HP}_{i,j,n}$ ) and feedstock requirement factors ( $\text{FRF}_{i,j,n}$ ) can be obtained from producers. It is *good practice* to avoid double counting with other sectors (Box 3.18). If data on feedstock consumption is also available, it is *good practice* to use the Tier 3b method. If data on actual hydrogen production is not available for a selection of plants, it should be considered to use production capacity as an estimate of production for these plants, or to use the Tier 2 method. It is *good practice* to use the method giving the lowest uncertainty. If plant specific feedstock requirement factors are not available, it is *good practice* to use default factors by production method and feedstock from Table 3.30. For carbon content factors ( $\text{CCF}_j$ ), default feedstock specific values from Table 1.3 in Vol.2, Chapter.1 or plant specific factors from producers could be used.

Information on the type of feedstock and production technology should be collected from the plants together with the production data and the factors, since the factors are specific to feedstock and production technology. If hydrogen production is not a *key category*, up to 5% [this percentage might be replaced with a default estimated percentage, based on the factor uncertainties] of national total hydrogen production volume may have unknown type of feedstock and production technology in the estimations. In this case, it is *good practice* to use the default general FRF and CCF.

If the feedstock contains biogenic components (f. ex. biodiesel, waste, etc.), the CO<sub>2</sub> emission ( $E_{\text{CO}_2}$ ) should be allocated partly to the hydrogen sector and partly to the IPPU memo item, relative to the respective fossil and biogenic carbon shares. The biogenic share should be obtained from the producers.

Recovered CO<sub>2</sub> is typically sold for use in other manufacturing industries, but could also be sent to permanent storages. Stored carbon is 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 material is available, it is *good practice* to assume that the material is pure carbon. It is *good practice* to exclude recovered CO<sub>2</sub> and stored carbon from the estimated emissions in the hydrogen production sector.

CO<sub>2</sub> recovered for use in other manufacturing industries, for example industrial CO<sub>2</sub> 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 include these emissions in the respective sectors.

### TIER 3B METHOD

The Tier 3b method uses feedstock consumption data from producers, together with data on recovery of CO<sub>2</sub> and stored amounts of carbon. The CO<sub>2</sub> emissions are estimated as follows:

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**EQUATION 3.47****CO<sub>2</sub> EMISSIONS FROM HYDROGEN PRODUCTION – TIER 3B**

$$E_{CO_2} = \sum_j (HRC_j \cdot CCF_j \cdot 44/12) - (R_{CO_2} + S_C \cdot 44/12)$$

Where:

 $E_{CO_2}$  = emissions of CO<sub>2</sub> (tonnes) $HRC_j$  = consumption of feedstock in production hydrogen as main product, feedstock  $j$  (tonnes) $CCF_j$  = carbon content factor, feedstock  $j$  (tonne C / GJ feedstock) $R_{CO_2}$  = CO<sub>2</sub> recovered (tonnes) $S_C$  = carbon stored (tonnes)

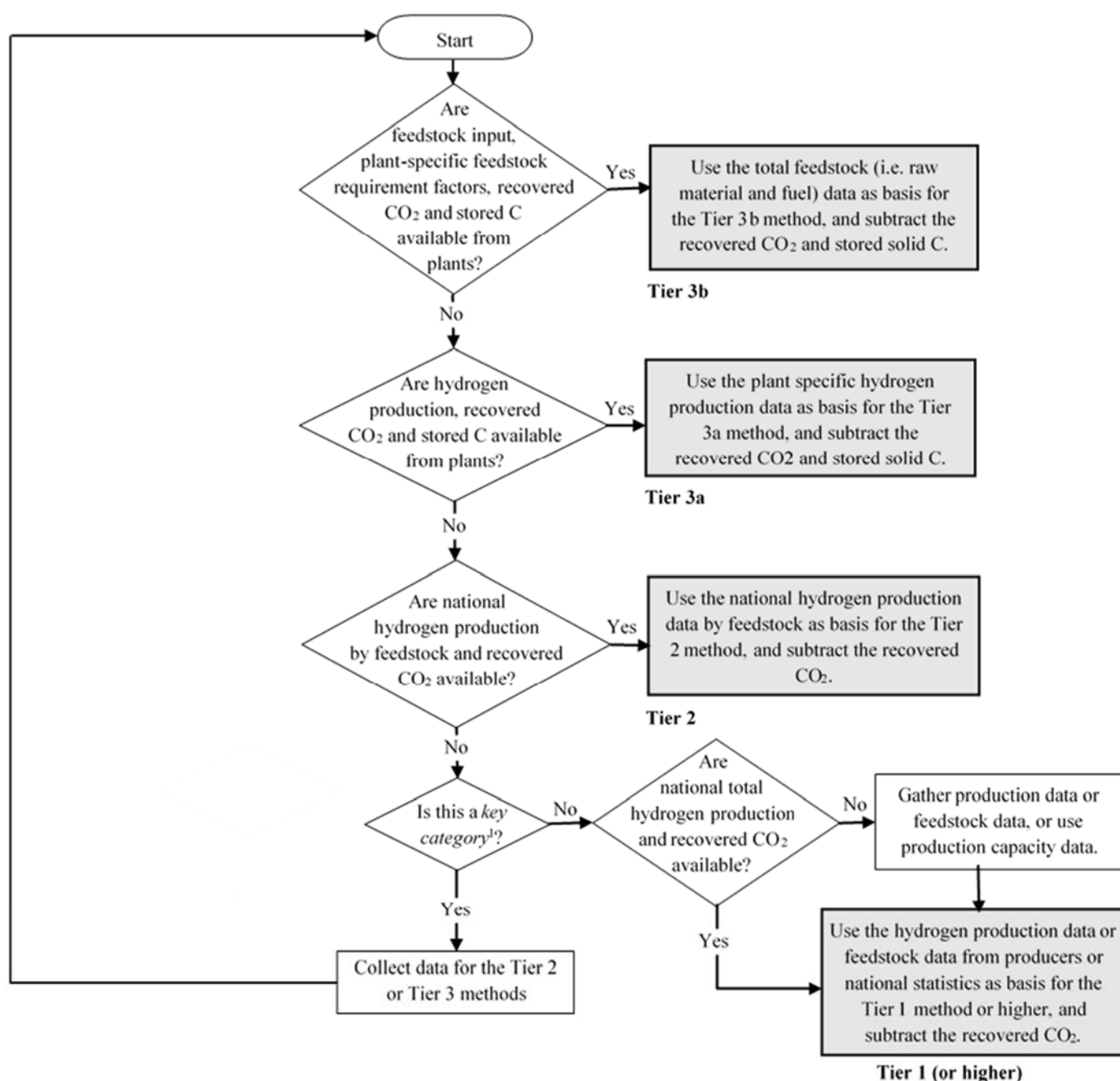
The feedstock consumption, by type, can be obtained from producers or national statistics. It is *good practice* to avoid double counting with other sectors (Box 3.18). Note that plant specific consumption data is not necessary in the Tier 3b method, since the all the feedstock is assumed to be converted to CO<sub>2</sub> emissions or stored as solid carbon. Default feedstock specific carbon content factors (CCF) are given in Table 1.3 in Vol.2, Chapter.1.

If the feedstock contains biogenic components (f. ex. biodiesel, waste, etc.), the CO<sub>2</sub> emission ( $E_{CO_2}$ ) should be allocated partly to the hydrogen sector and partly to the IPPU memo item, relative to the respective fossil and biogenic carbon shares. The biogenic share should be obtained from the producers.

Recovered CO<sub>2</sub> is typically sold for use in other manufacturing industries, but could also be sent to permanent storages. Stored carbon is 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 material is available, it is *good practice* to assume that the material is pure carbon. It is *good practice* to exclude recovered CO<sub>2</sub> and stored carbon from the estimated emissions in the hydrogen production sector.

CO<sub>2</sub> recovered for use in other manufacturing industries, for example industrial CO<sub>2</sub> 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 include these emissions in the respective sectors.

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**Figure 3.20** Decision tree for estimation of CO<sub>2</sub> emissions from hydrogen production

Note 1: 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

#### TIER 1 METHOD

In the Tier 1 method, it is *good practice* to use the default feedstock requirement factor (FRF) and carbon content factor (CCF) in table 3.30. These default values often represent midpoint or mean values of data sets (as determined by expert analysis).

The feedstock requirement factor converts the production of hydrogen into the corresponding consumption of feedstock (raw material and fuel). The carbon content factor is used to convert the amount of feedstock (i.e. raw material and fuel) in GJ into tonnes of carbon. The default factors are the average factors for the most common feedstock types, weighted according to the global production.

#### TIER 2 METHOD

The feedstock requirement factor (FRF) converts the production of hydrogen into the corresponding consumption of feedstock (i.e. raw material and fuel). The carbon content factor (CCF) is used to convert the amount of feedstock in GJ into tonnes of carbon.

In the Tier 2 method, it is *good practice* to use feedstock specific feedstock requirement factors and carbon content factors. Default factors for selected types of feedstock are provided in Table 3.30 in this chapter and Table 1.3 in Vol.2, Chapter.1.

See Tier 1 method for more details.

#### TIER 3 METHODS

##### Tier 3a

The feedstock requirement factor (FRF) converts the production of hydrogen into the corresponding consumption of feedstock (i.e. raw material and fuel). The carbon content factor (CCF) is used to convert the amount of feedstock in GJ into tonnes of carbon. If plant-level factors are not available, it is *good practice* to use default feedstock and process specific feedstock requirement factors and carbon content factors. Default factors for selected production processes and types of feedstock are provided in Table 3.30 in this chapter and Table 1.3 in Vol.2, Chapter.1.

See Tier 1 method for more details.

##### Tier 3b

The carbon content factor (CCF) is used to convert the amount of feedstock (i.e. raw material and fuel) in GJ into tonnes of carbon. Default CCFs for selected types of feedstock are given in Table 3.30 in this chapter and Table 1.3 in Vol.2, Chapter.1.

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TABLE 3.30 DEFAULT FEEDSTOCK REQUIREMENTS AND CARBON CONTENT FACTORS FOR HYDROGEN PRODUCTION <sup>1</sup>				
Production Process	Feedstock requirement (GJ feedstock/tonne H <sub>2</sub> ) ± Uncertainty <sup>1</sup>	Carbon content factor (tonne C / GJ feedstock)		
Fuel reforming		Default	Lower	Upper
Natural gas reforming	160 (± 10%)	15.3	14.8	15.9
Liquified petroleum gas reforming	165 (± 15%)	17.2	16.8	17.9
Naphtha reforming	165 (± 15%)	20.0	18.9	20.8
Biofuel reforming, other liquids (bioethanol)	176 (± 20%)	21.7	18.3	26.0
Gasification				
Coal gasification	210 (± 15%)	25.8	23.8	27.6
Plastic gasification	185 (± 10%)	20.0	[XXX]*	[XXX]*
Mixed waste gasification (non-biomass fraction)	273 (± 15%)	25.0	20.0	33.0
Wood waste gasification	260 (± 10%)	30.5	25.9	36.0
Wood sludge gasification	194 (± 15%)	30.5	25.9	36.0
Black liquor gasification	149 (± 10%)	26.0	22.0	30.0
General				
Default	171 (± 30%)**	18.3***	14.8***	27.6***
<sup>1</sup> 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. Sources: Cormos (2011); DOE (2017); Geissler, et al. (2001); GREET (2013); Iwasaki (2003); JARI (2011); JRC (2014); Schiebahn et al. (2015); Sorensen (2011); The Pacific Northwest National Laboratory (2017); Wallman et al. (1998).				

[\* - to be established later ;

\*\* - estimated by weighted average of natural gas (49%), LPG/naphtha (29%) and coal (18%), based on global production statistics. Uncertainty set to cover the ranges of these three feedstock types, which are by far the most common at present ;

\*\*\* - Estimated by weighted average of natural gas (49%), LPG/naphtha (29%) and coal (18%), based on global production statistics. Lower range from natural gas, upper range from coal]

### 3.11.2.3 CHOICE OF ACTIVITY DATA

#### TIER 1 METHOD

National hydrogen production data on a total level (HP) may be used in the Tier 1 method. If production data (or feedstock data) is not available, 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 production capacity by a capacity utilisation factor of 80 percent ± 10 percent (i.e., a range of 70-90 percent). The same capacity utilisation factor should be applied to each year of the time-series. [a typical capacity utilization in hydrogen production will be considered later. The values are copied from the ammonia chapter]. It can be assumed that the same type of material is used for both raw material and fuel in a given production method. Emissions reported in other sectors should be excluded to avoid double counting (Box 3.18).

It is *good practice* to exclude recovered (i.e. delivered to other sectors for use, or permanently stored) CO<sub>2</sub> from the estimated emissions. If no data on recovered CO<sub>2</sub> could be obtained, it is *good practice* to assume that the recovery is zero. The biogenic share should be obtained, to estimate the CO<sub>2</sub> emissions to be reported in the IPPU memo item. If the biogenic share cannot be estimated, it is *good practice* to assume that all feedstock is fossil.

#### TIER 2 METHOD

The Tier 2 method requires national level data on the amount of hydrogen produced, split by type of feedstock. It is *good practice* to avoid double counting (Box 3.18). It can be assumed that the same type of material is used for both raw material and fuel in a given production method. If an adequate split of the production data by type of feedstock is unavailable, it is *good practice* to use the Tier 1 method.

It is *good practice* to exclude recovered (i.e. delivered to other sectors for use, or permanently stored) CO<sub>2</sub> from the estimated emissions. If no data on recovered CO<sub>2</sub> could be obtained, it is *good practice* to assume that the

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recovery is zero. The biogenic share should be obtained, to estimate the CO<sub>2</sub> emissions to be reported in the IPPU memo item. If the biogenic share cannot be estimated, it is good practice to assume that all feedstock is fossil.

**TIER 3A METHOD**

The Tier 3a method requires plant-level data on hydrogen production, by production method and type of feedstock. If data on hydrogen production is not available for a selection of plants, it should be considered to use production capacity as an estimate of production for these plants, or to use the Tier 2 method. It is *good practice* to use the approach giving the lowest uncertainty.

Information on the type of feedstock should be collected from the plants together with the production data and the factors, since the factors are feedstock specific. If hydrogen production is not a *key category*, up to 5% [this percentage might be replaced with a default estimated percentage, based on the factor uncertainties] of national total hydrogen production volume may have unknown feedstock type in the estimations.

It is *good practice* to exclude recovered CO<sub>2</sub> and stored solid carbon from the estimated emissions. If no data on recovered CO<sub>2</sub> and stored solid carbon could be obtained from the producers, it is *good practice* to assume that the recovery and stored solid carbon are zero. The biogenic share should be obtained from the producers, to estimate the CO<sub>2</sub> emissions to be reported in the IPPU memo item. If the biogenic share cannot be estimated, it is *good practice* to assume that all feedstock is fossil.

**TIER 3B METHOD**

The Tier 3b method requires plant-level data on feedstock consumption, by type of feedstock. Data on feedstock type and consumption, together with recovered CO<sub>2</sub>, stored carbon and share of biogenic fuel, should be obtained from producers. If plant-level data on feedstock type and consumption is available, it is *good practice* to prefer the Tier 3b method over the Tier 3a method, due to lower uncertainty. If not, it should be considered to use the Tier 3a method or lower Tier methods. 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.

It is *good practice* to exclude recovered CO<sub>2</sub> and stored solid carbon from the estimated emissions. Where 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. If no data on recovered CO<sub>2</sub> and stored solid carbon could be obtained from the producers, it is *good practice* to assume that the recovery and stored solid carbon are zero. The biogenic share should be obtained from the producers, to estimate the CO<sub>2</sub> emissions to be reported in the IPPU memo item. If the biogenic share cannot be estimated, it is *good practice* to assume that all feedstock is fossil.

Although data on hydrogen production is not used in the calculation under the Tier 3b method it also needs to be collected from producers and reported for use in the QA/QC routines.

**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 practise* to report the lower Tier as the applied method, except in cases described in section 3.11.2.3. 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 must be excluded from hydrogen production (Box 3.18).

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**Box 3.18**  
**DOUBLE COUNTING**

- In order to avoid double counting, when hydrogen is produced as a by-product or intermediate product, it is *good practice* to report the CO<sub>2</sub> emissions in the sector of the main product.
- 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. These sectors include refineries and ammonia production.
- Conversely, emissions from production of hydrogen reported in the **Hydrogen production** sector must be excluded from other sectors.
- Fuel consumed as part of the production process should be reported in the **Hydrogen production** sector. Fuel consumed for other purposes should be reported in other sectors. For instance, fuel used for heating buildings should be reported in the Energy sector (stationary combustion).
- The quantity of recovered CO<sub>2</sub> includes quantities delivered for downstream use in other manufacturing industries. The recovered quantity must be subtracted from the estimated emissions in the Hydrogen production sector, while the corresponding emissions of CO<sub>2</sub> from downstream use should be accounted for in the corresponding sectors.

### 3.11.2.5 DEVELOPING A CONSISTENT TIME SERIES

CO<sub>2</sub> emissions should be recalculated 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 is not available, including plant-specific data for hydrogen production, consumed feedstock, recovered CO<sub>2</sub> and stored C, 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 production 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 or plant) as the activity data. In case of plant level data, the uncertainty should be lower than uncertainty values associated with default values.

Fuel requirement factors (FRFs): Uncertainty in the default fuel requirement factors 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 feedstock is burnt for 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. Estimation methods using fuel requirement factors (Tier 1, 2 and 3a) have higher overall uncertainty than methods not using the fuel requirement factors (Tier 3b), *ceteris paribus*.

Carbon content factors (CCFs): Uncertainty in the default carbon content factors 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. Small uncertainties may arise from variation in composition and energy content of the specific material used as feedstock (f. ex. ethane in natural gas), while larger uncertainties arise when the carbon content factor represents a feedstock 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.

In the Tier 1, Tier 2 and Tier 3a methods, it is assumed that the same type of material is used for both raw material and fuel in a given production method. If different materials are being used for raw material and fuel, the uncertainty will increase accordingly. An increase of  $\pm 10$  percentage points [a value will be elaborated] should be used as a default *increase* in the overall uncertainty, or country specific uncertainties could be used if available.



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If no information is available on the type of feedstock, and hence the highest default CCF value among the feedstock types used in the member state is used for the entire production (option in Tier 1), the uncertainty will increase in the downward direction. An increase of 20 percentage points [a value will be elaborated] should be used as a default *increase* in the downward uncertainty, or country specific uncertainties could be used if available.

The biogenic share is considered to have a negligible uncertainty, as it is a low value and based on reported data.

### 3.11.3.2 ACTIVITY DATA UNCERTAINTIES

Where activity data is obtained from plants, uncertainty estimates can be obtained from producers. This activity data is likely to be highly accurate (i.e., with uncertainty as low as  $\pm 2$  percent). It includes uncertainty estimates for hydrogen production (Tier 1, 2 and 3a) or feedstock use (Tier 3b), CO<sub>2</sub> recovered and carbon stored. 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  $\pm 5$  percent can be used [a value will be checked].

If plant-specific data is not available for all years in the time series, and current data is 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 value of  $\pm 20$  percent can be used [a value will be elaborated] .

## 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. [Additional QA/QC routines might be proposed in the SOD.]

#### Comparison of emission factors

Inventory compilers should check if the estimated factors are within the range of default factors provided for the appropriate Tier method, and also ensure that the emission factors are consistent with the values derived from analysis of the process chemistry. For example, the CO<sub>2</sub> generation rate based on natural gas should not be less than 5.46 tonnes of CO<sub>2</sub> per tonne of hydrogen produced [method:  $44.011 \text{ tonnes CO}_2 / 8.064 \text{ tonnes H} = 5.46 \text{ tonnes of CO}_2 \text{ per tonne of H}_2 \text{ produced, based on molar weights of 12.011 (C), 16.00 (O), 1.008 (H) and 100\% \text{ production yield (i.e. no fossil fuel use or loss)}$ ]. If the emission factors are outside of the estimated ranges, it is *good practice* to assess and document the plant-specific conditions that account for the differences.

#### 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;
- Tier 3b only: Activity data comprising both input data (feedstock consumption) and output data (hydrogen production).

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



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1490 inventory report. However, the inventory should include summaries of methods used and references to source data  
1491 such that the reported emissions estimates are transparent and steps in their calculation may be retraced.

1492 Much of the production and process data is considered proprietary by operators, especially where there are only a  
1493 small number of plants within a country. It is *good practice* to apply appropriate techniques, including aggregation  
1494 of data, to ensure protection of confidential data. Guidance on managing confidential data is provided in Section  
1495 2.2, Volume 1.

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**References****SECTIONS 3.2 - 3.8**

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