Introduction to Emission Factors

Lys Draper - Senior Consultant / Semiconductor SME

Presenters profile

Lys Draper

Senior Consultant | Trinity Consultants

- B.S. and M.S. Chemical Engineering – University of Utah
- Started at Trinity in 2024
- Air quality, toxic release inventory, GHG reporting
- Working in semiconductor fabs since 2015 in process engineering and facilities
- One of Trinity's subject matter experts for the semiconductor industry

Contact Info

Office Location: Phoenix, AZ

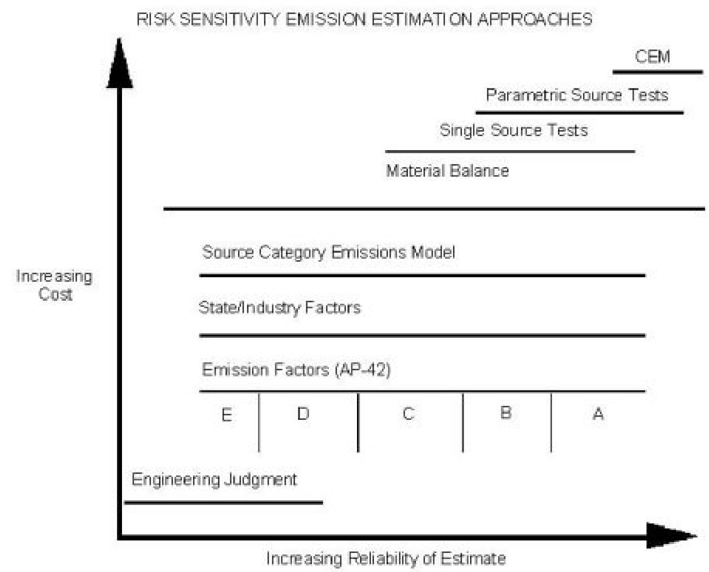
Telephone: (602) 274-2900 x 5312

lysdraper@trinityconsultants.com

What is emissions estimation?

And what is it for?

EPA Preferred Emissions Estimation Methods[2]



- Continuous Emissions Monitoring System (CEMS)
- Stack Testing
- Vendor Guarantees
- Stack Test Data from Similar Facilities
- Material Balance Calculations
- Other direct measurement
- AP-42 Emissions Factors
  - When source-specific emissions or other more reliable approaches are unavailable, AP-42 emissions factors may be the only way to estimate emissions. AP-42 emissions factors should only be used as a last resort.

2. EPA, Best Practices for Estimating Emissions Using Emissions Factors for Clean Air Act Permitting, 2021, https://www.epa.gov/system/files/documents/2022-02/emissions-factors-best-practices_0.pdf

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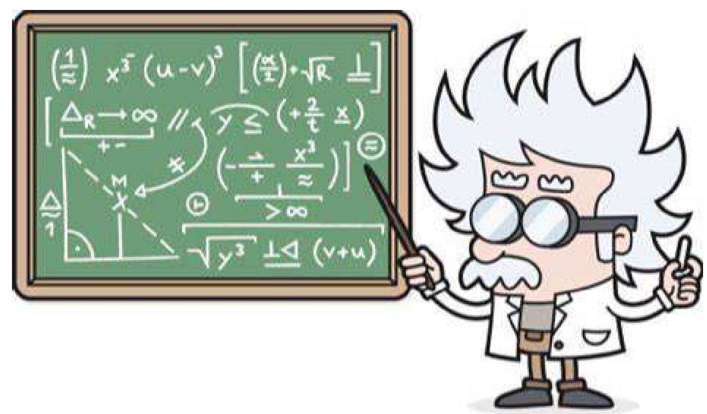
What is an emission factor?

"A numerical value that represents the quantity of a pollutant released to the atmosphere with an activity associated with the release of that pollutant. These factors are usually expressed as the weight of pollutant divided by a unit weight, volume, distance, or duration of the activity emitting the pollutant." [1]

1. EPA, Basic Information of Air Emissions Factors and Quantification, 2024. https://www.epa.gov/air-emissions-factors-and-quantification/basic-information-air-emissions-factors-and-quantification

Purpose of Emission Factors

- Used to represent long-term (e.g., annual) average emissions
- Used to estimate the emissions generated by each emission-generating unit for:
  - Potential-to-Emit (PTE) calculations are used to compare against permitting thresholds
  - Annual emissions inventories
  - Greenhouse gas (GHG) emissions inventories and reporting



Emission Factor Equation

- General equation for emissions estimation[2]
  - $E = A * EF * (1 - ER)$
    - *E* = Emissions
    - *A* = Activity Rate
    - *EF* = Emission Factor
    - *ER* = Overall Emission Reduction Efficiency (%)
- If the activity has no control efficiency, the ER is 0

2. EPA, Best Practices for Estimating Emissions Using Emissions Factors for Clean Air Act Permitting, 2021, https://www.epa.gov/system/files/documents/2022-02/emissions-factors-best-practices_0.pdf

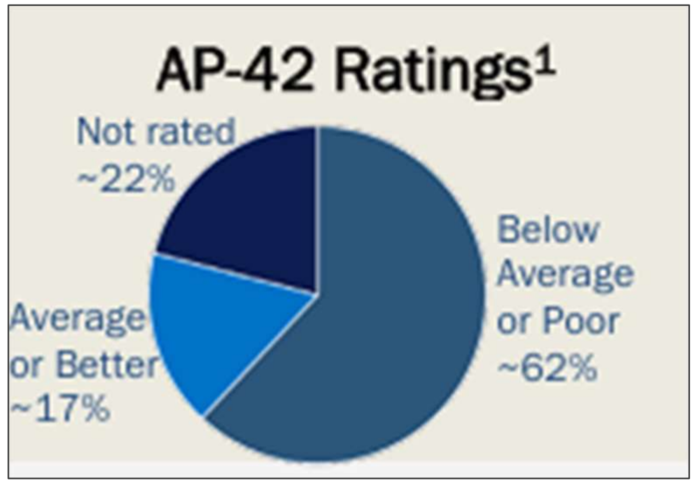
Emissions Factor Uncertainty[3]

- Because emission factors are derived through averages there is an inherent error within them.
- Hazardous Air Pollutants (HAPs) typically have the highest uncertainty.
- When emission factors have a greater number of tests to derive them, they have a lower uncertainty ratio.

3. RTI International, Emissions Factor Uncertainty Assessment, 2007, https://www.epa.gov/sites/default/files/2020-11/documents/ef_uncertainty_assess_draft0207s.pdf

Emissions Factor Ratings in AP-42

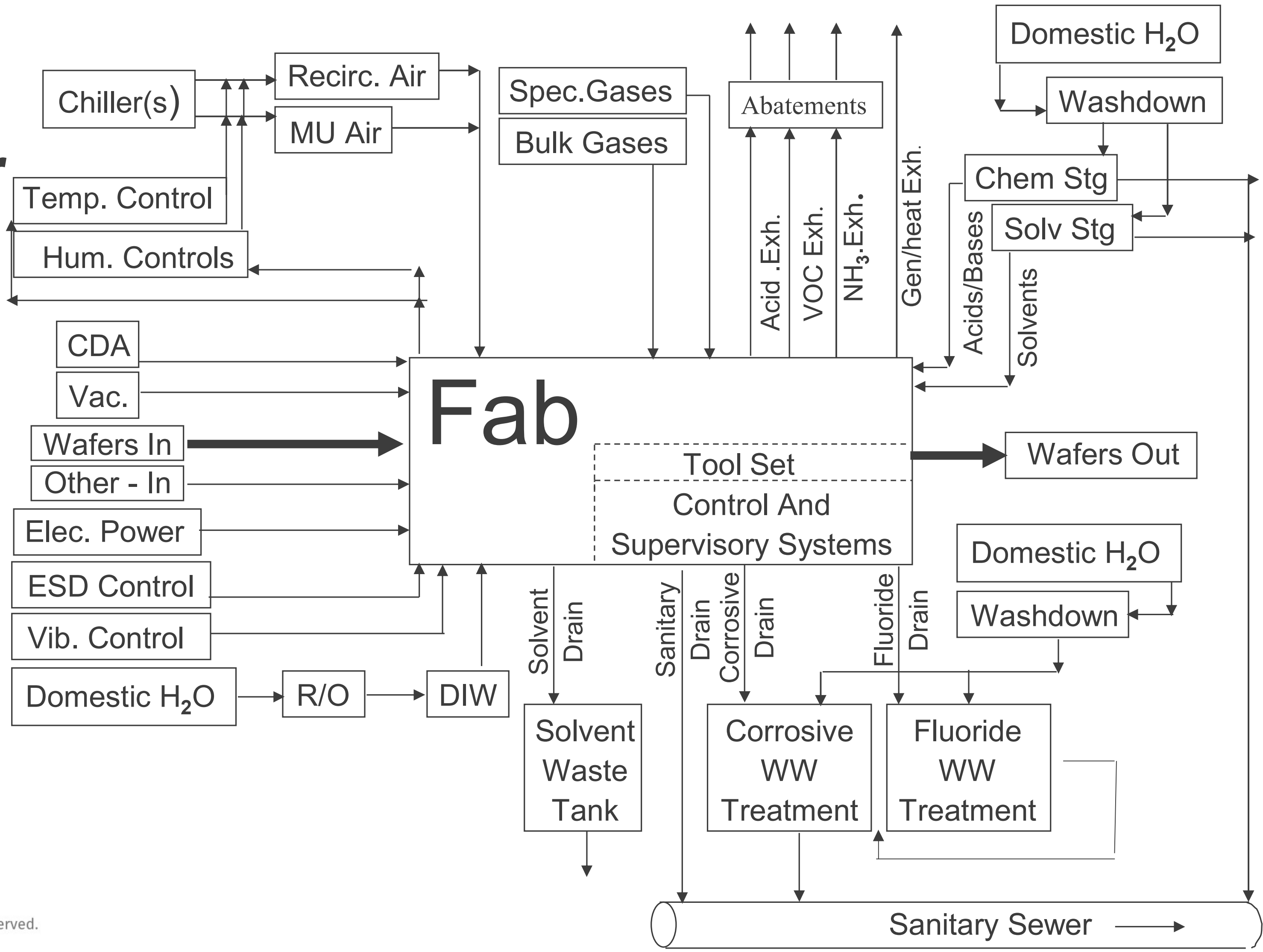
- A-E[4]
  - A: Excellent
  - B: Above Average
  - C: Average
  - D: Below Average
  - E: Poor

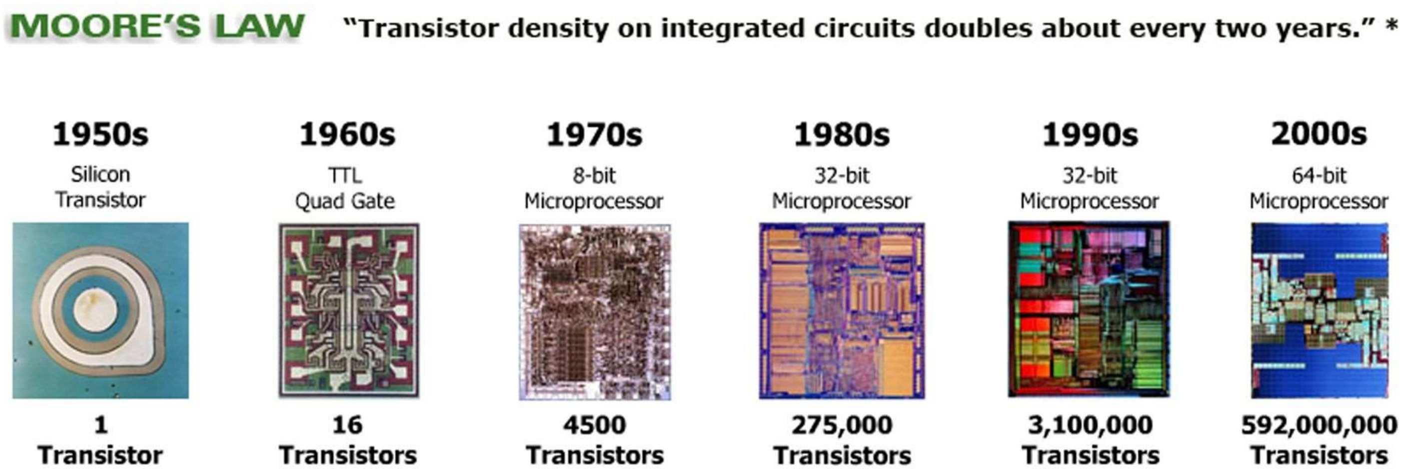


4. EPA, Best Practices for Estimating Emissions Using Emissions Factors for Clean Air Act Permitting, 2021, https://www.epa.gov/system/files/documents/2022-02/emissions-factors-best-practices_0.pdf

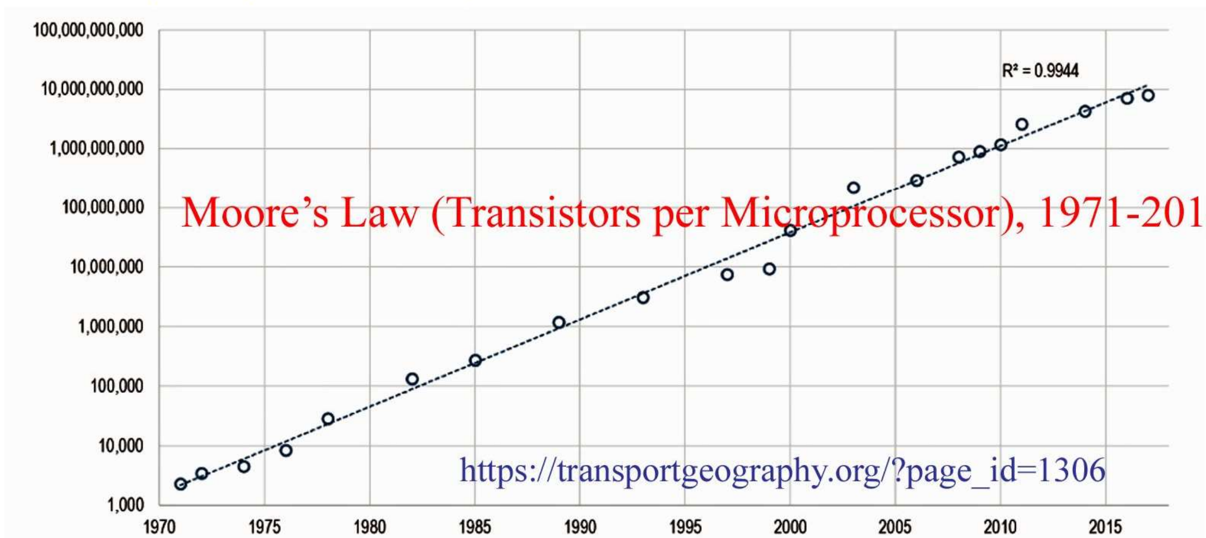
Emission Factors in the Semiconductor Industry

- Historical use and applications
  - Many of these processes need their own emissions estimates
  - Chemical reactions and byproducts
  - Rule 338 Revisions - NOx emissions from POU abatement





https://impulseseee.wordpress.com/2017/08/24/evolution-of-transistors-2/



Moore's Law (Transistors per Microprocessor), 1971-2018

https://transportgeography.org/?page_id=1306

Emission Factors in the Semiconductor Industry

- IPCC and EPA have published GHG EFs specific to the industry
- There are no published EFs for other pollutants specific to semiconductor processes
  - Instead, facilities rely on site-specific test data and/or mass balance estimates based on industry experience

TABLE I-4 TO SUBPART I OF PART 98—DEFAULT EMISSION FACTORS (1-U_{IJ}) FOR GAS UTILIZATION RATES (U_{IJ}) AND BY-PRODUCT FORMATION RATES (B_{IJK}) FOR SEMICONDUCTOR MANUFACTURING FOR 300 mm AND 450 mm WAFER SIZE

Process type/sub-type	Process gas i											
	CF_4	C_2F_6	CHF_3	CH_2F_2	CH_3F	C_3F_8	C_4F_8	NF_3	SF_6	C_4F_6	C_5F_8	C_4F_8O
ETCHING/WAFER CLEANING												
1-U_i	0.65	0.80	0.37	0.20	0.30	0.30	0.18	0.16	0.30	0.15	0.10	NA
BCF_4	NA	0.21	0.076	0.060	0.0291	0.21	0.045	0.044	0.033	0.059	0.11	NA
BC_2F_6	0.058	NA	0.058	0.043	0.009	0.018	0.027	0.045	0.041	0.062	0.083	NA
BC_4F_8	0.0046	NA	0.0027	0.054	0.0070	NA	NA	NA	NA	0.0051	NA	NA
BC_3F_8	NA	NA	NA	NA	NA	NA	NA	NA	NA	NA	0.00012	NA
$BCHF_3$	0.012	NA	NA	0.057	0.016	0.012	0.028	0.023	0.0039	0.017	0.0069	NA
BCH_2F_2	0.005	NA	0.0024	NA	0.0033	NA	0.0021	0.00074	0.000020	0.000030	NA	NA
BCH_3F	0.0061	NA	0.027	0.0036	NA	0.00073	0.0063	0.0080	0.0082	0.00065	NA	NA

Choosing Emission Quantification Methodologies

- Testing Data
- Facility mass balance
- Engineering estimates
  - Chemical properties

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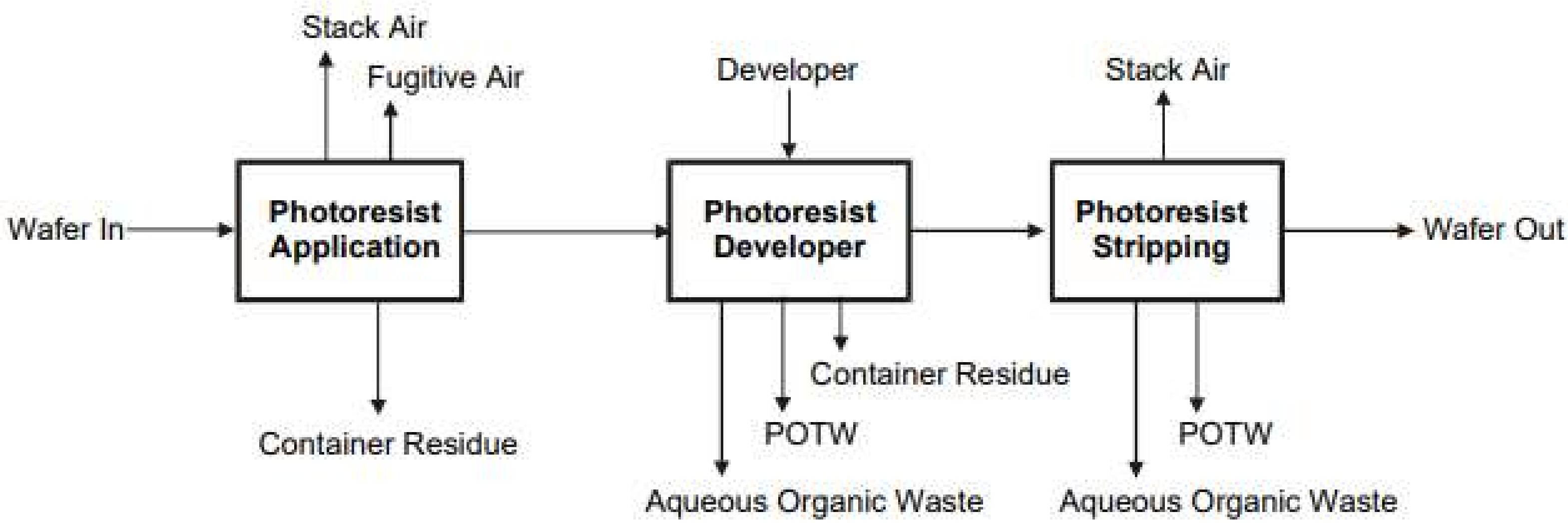
Example: Mass Balance



$$\begin{bmatrix}\text{rate of mass}\\ \text{accumulation within}\\ \text{system boundaries}\end{bmatrix} = \begin{bmatrix}\text{rate of mass flow}\\ \text{into system}\end{bmatrix} - \begin{bmatrix}\text{rate of mass flow}\\ \text{out of system}\end{bmatrix}$$

$$\dot{m} = \sum_{inlets} \dot{m}^{in} - \sum_{outlets} \dot{m}^{out}$$

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Example: Test Data and Mass Balance

Anhydrous ammonia is used to deposit a layer of silicon nitride during wafer fabrication.

- 17,000 pounds of ammonia was used in 1 year
- 20 percent of the total ammonia used is deposited on the wafer
- The rest goes to a scrubber with 90% control efficiency

Point source air emissions = 17,000 (lb/year) x (amnt not depped) x (1-ctrl eff)

= 17,000 (lb/year) x (1 - 0.2) x (1 - 0.9) = 1,360 lb/yr

Amount sent to wastewater = 17,000 (lb/yr) x (amnt not depped) x (ctrl eff)

= 17,000 (lb/yr) x (1 - 0.2) x (0.9) = 12,240 lb/yr

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Example: Engineering Estimates

Example - Cleaning

Your facility uses methanol as a cleaner in a wet bath that is operated 5 days a week, 50 weeks per year, for 8 hours each day.

You can estimate methanol emissions using mass transfer kinetics and the following equation (from *Estimating Releases and Waste Treatment Efficiencies for the Toxic Chemical Release and Inventory Form*):

$$W_x = \frac{Mw_x \times K \times A \times P_{vap,x}}{R \times T}$$

where:	W_x	=	Evaporation rate of pollutant X (lb/sec)
	Mw_x	=	Molecular weight of pollutant X (lb/lb-mole)
	K	=	Gas-phase mass transfer coefficient (ft/sec)
		=	$0.00438 \times U^{0.78} \times (18/Mw_x)^{1/3}$
	U	=	Wind speed (miles/hr)
	A	=	Surface area (ft^2)
	$P_{vap,x}$	=	Vapor pressure of pollutant X (psia)
	R	=	Ideal gas constant (10.73 psia × ft^3/°R × lb-mole)
	T	=	Temperature of bath (°R)

Given the following data:

Mw_x	=	32 lb methanol/lb-mole
U	=	1.7 miles/hr (default value)
A	=	1 ft^2 (assumed surface area of your bath)
$P_{vap,x}$	=	1.91 psia (pure vapor pressure of methanol)
T	=	533°R, °R = (9/5) × (°C + 273)
R	=	10.73 psia × ft^3/°R × lb-mole

First, calculate the mass transfer coefficient, K:

$$K = 0.00438 \times U^{0.78} \times (18/Mw_x)^{1/3}$$
$$= 0.00547 \text{ (ft/sec)}$$

Then, calculate W_x:

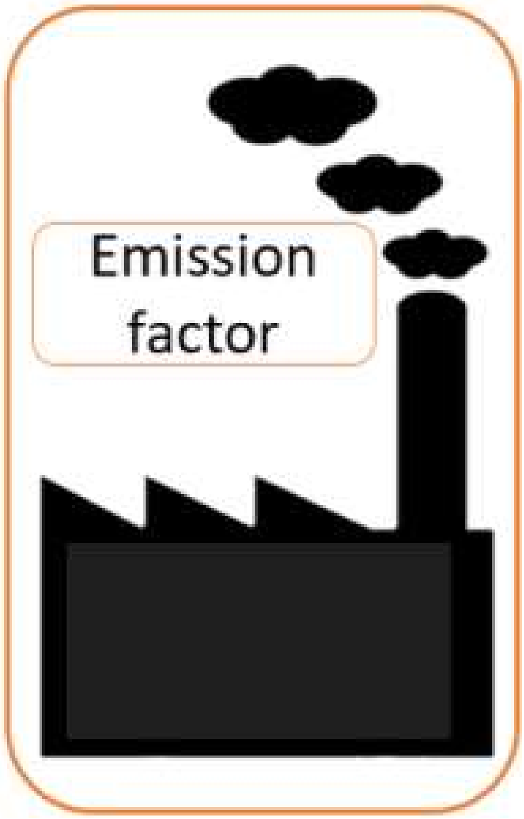
$$W_x = \frac{Mw_x \times K \times A \times P_{vap,x}}{R \times T}$$

$$= (32 \text{ lb/mole}) \times (0.00547 \text{ ft/sec}) \times (1 \text{ ft}^2) \times (1.91 \text{ psia}) \div (10.73 \text{ psia ft}^3) \div (°R \times \text{lb-mole}) \div (533°R)$$

$$= 5.84 \times 10^{-5} \text{ lb/sec}$$

Developing Emission Factors

- Site specific
- Data collection and analysis
- When to use existing factors
- Adding conservatism



Conservative Emission Estimates Based On Phase

- Solids at room temperature can be conservatively assumed to be partially emitted in trace quantities.
- Liquids at room temperature can be assumed to partially evaporate based on their chemical properties and/or test data.
- 100% of the mass of gases at room temperature can be assumed to either be emitted directly or react into another gas.
  - If data is available for the efficiency of processes such as CVD, that can be accounted for to refine emissions estimates.

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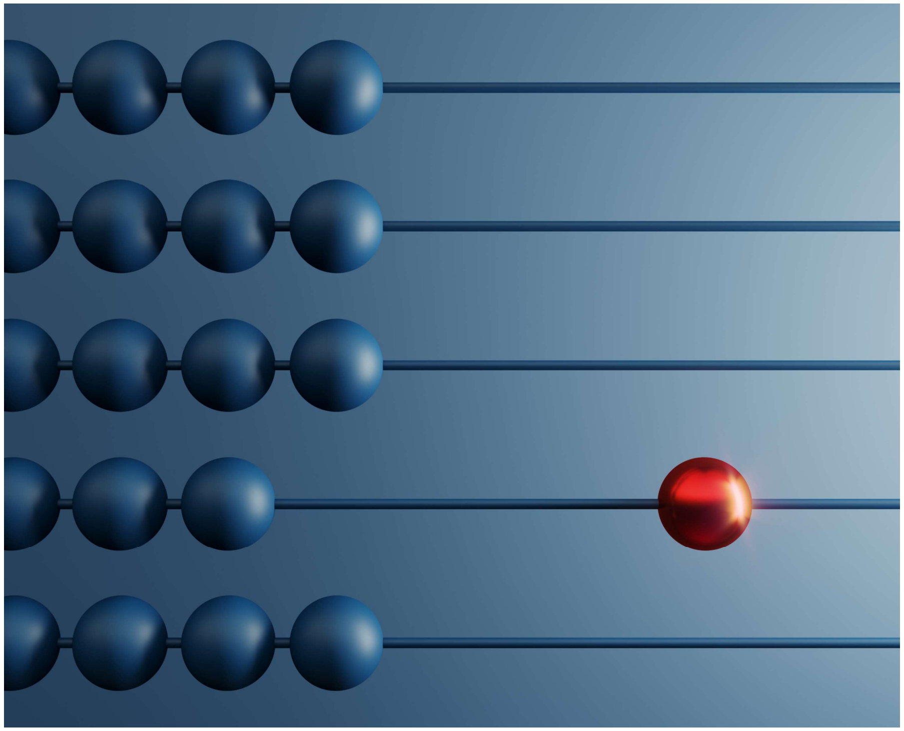
More Conservative Assumptions

- Assume compounds that enter burners fully oxidize to NO_2, CO_2, SiO_2, etc.
- Use testing data to refine emission factor values
- Err on the conservative side to make sure emissions are not being underestimated



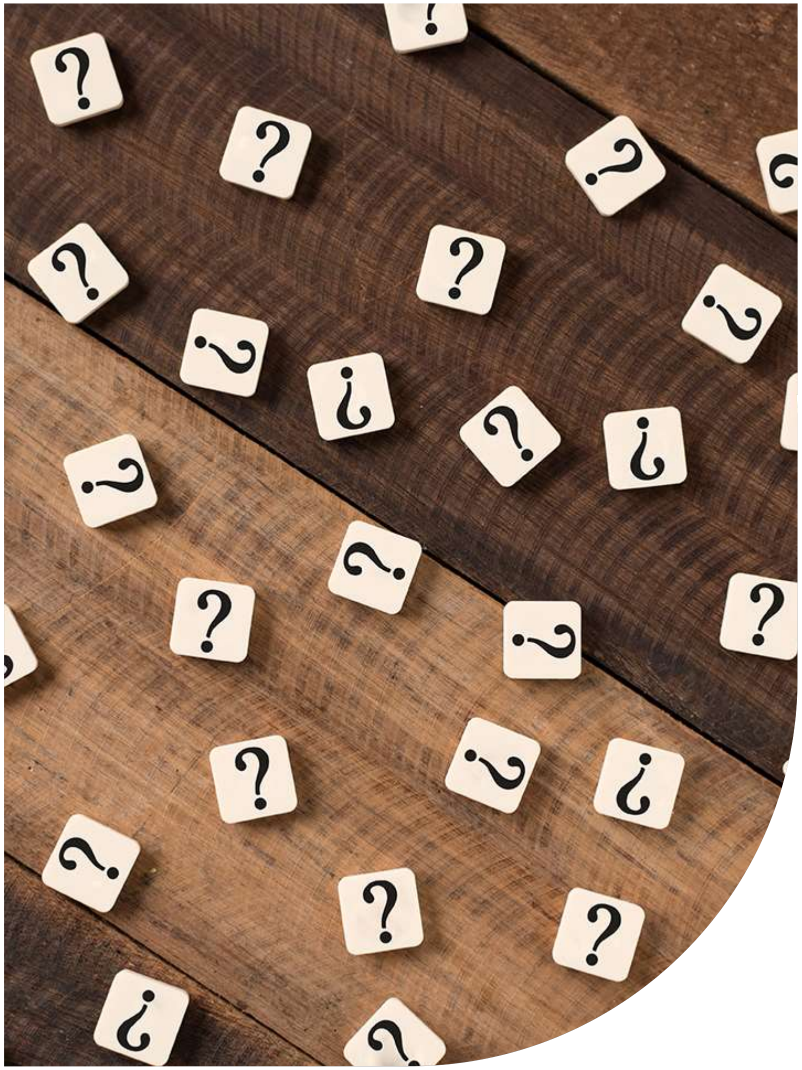
Stack Testing Plan Development

- Best practices
  - Collect data that will help you determine reliability of emission factors
    - Production data (wafer moves, wafer starts)
    - Chemical usage data
    - Equipment uptime
- Use data to define emission factors
- Repeat testing and refine estimates

Conclusion

- There are many ways for estimating emissions
  - Testing data is generally preferred
  - Stack testing, chemical properties, and engineering estimates can be used together
- Collect data, refine emission factors, and repeat
- Emission factors aren't a perfect estimate
- Conservative assumptions help ensure regulatory compliance and sustainable practices
  - When in doubt, account for it

Questions



Optical Remote Sensing Technologies

Emissions Estimation by “Other direct measurement”

FTIR

Tunable Diode Laster

UV Differential Optical Absorption Spectroscopy

Thermal Infrared Cameras

Particulate Matter LIDAR

Other spectroscopy methods

EPA Handbook: Optical and Remote Sensing for Measurement and Monitoring of Emissions Flux of Gases and Particulate Matter, 2018. [gd-52v.2.pdf]

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