CHEM 1101B- Chemistry for Engineers

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HS (Health Sciences) 1301
Mondays & Wednesdays 8:35am - 9:55am

Lecture 15: Stoichiometry

Please feel free to introduce yourself to your neighbors– name, pronouns, a hobby, etc.

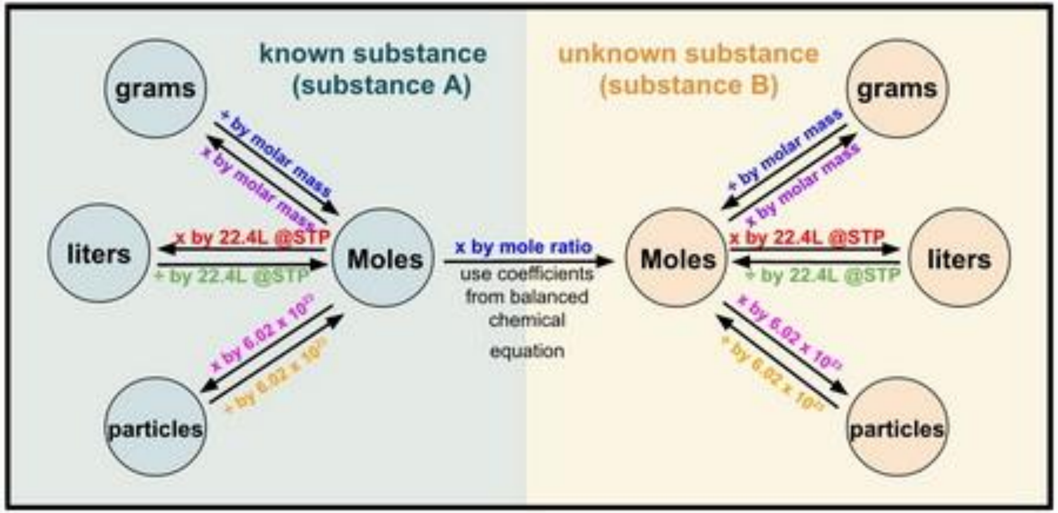
and/or

Answer first wooclap question

Learning outcome for Topic 15: Stoichiometry

Learning Outcomes:

- Describe the rules of conservation of atoms in chemical reactions
- Predict the relative amounts of reagents consumed and leftover during chemical equations
- Carry out stoichiometry calculations with limiting reagents and specific yields



Chemical Reactions

The breaking of at least one existing chemical bond in the reagents and/or the formation of at least one new chemical bond in the products.

Example: Many modern rocket fuels are solid mixtures of substances combined in carefully measured amounts and ignited to yield a thrust-generating chemical reaction.

https://boisestate.pressbooks.pub/chemistry/chapter/intro-7/

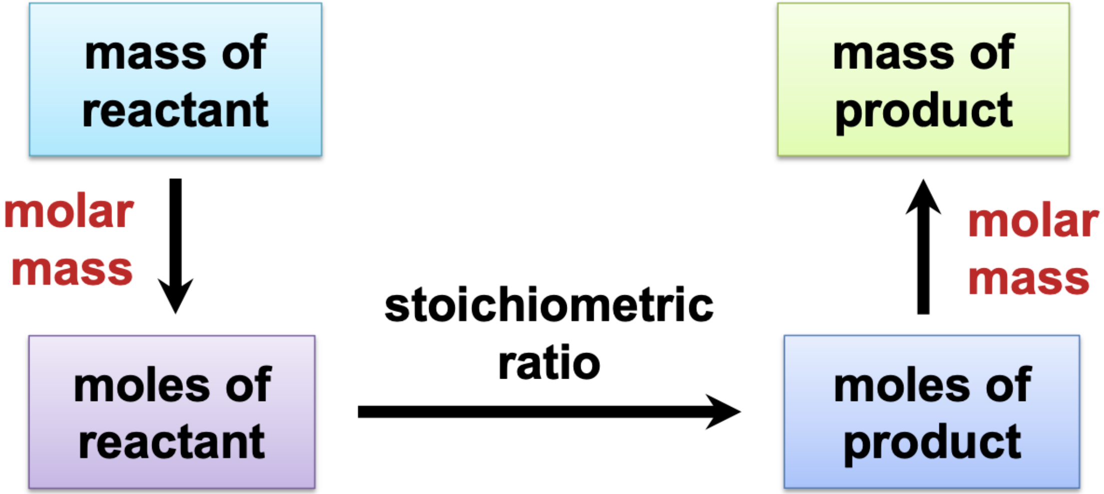
Stoichiometry

- The study of the quantitative aspects of a chemical reaction.
- if the quantity of reactant is known, it is possible to find the
- quantity of product that will be formed (or vice-versa)
- to simplify the process, we use the mole method:

1 mole → defined by the number of atoms in 12 g of pure 12C

Avogadro's number = N_A = 6.022×10^{23} units in one mole

Molar mass = the mass of 1 mole of that substance



Strategy for balancing equations

- Balance elements that occur in only one compound on each side first. Start with most complex compounds.
- Balance free elements last.
- Do not alter chemical formulas of compounds.
- Fractional coefficients are acceptable and can be cleared at the end by multiplication.

e.g. Balance:

$$Fe_3O_4 + HCl + Cl_2 \rightarrow FeCl_3 + H_2O + O_2$$

Practice: balancing equations

Balance free elements last:

$Fe_2O_3 + C \rightarrow FeO + CO$

If an element is in two different compounds on the same side of the equation, save it for last:

$C_4H_{10} + O_2 \rightarrow CO_2 + H_2O$

Rule of 2:3 (or 3:4)

$Fe_2O_3 + C \rightarrow Fe + CO_2$

Fractions vs. integers

$C_4H_{10} + O_2 \rightarrow CO_2 + H_2O$

Molecular ions

$Ca_3(PO_4)_2 + H_2SO_4 \rightarrow CaSO_4 + H_3PO_4$

Practice: balancing equations

Example: Ammonium nitrate (NH_4NO_3) explodes when it is heated above 300 °C. The products are three gases: molecular nitrogen, molecular oxygen, and steam (water vapour). Write a balanced equation for the explosion of ammonium nitrate.

$$\_\_\_NH_4NO_3 \rightarrow \_\_\ N_2 + \_\_\ H_2O + \_\_O_2$$

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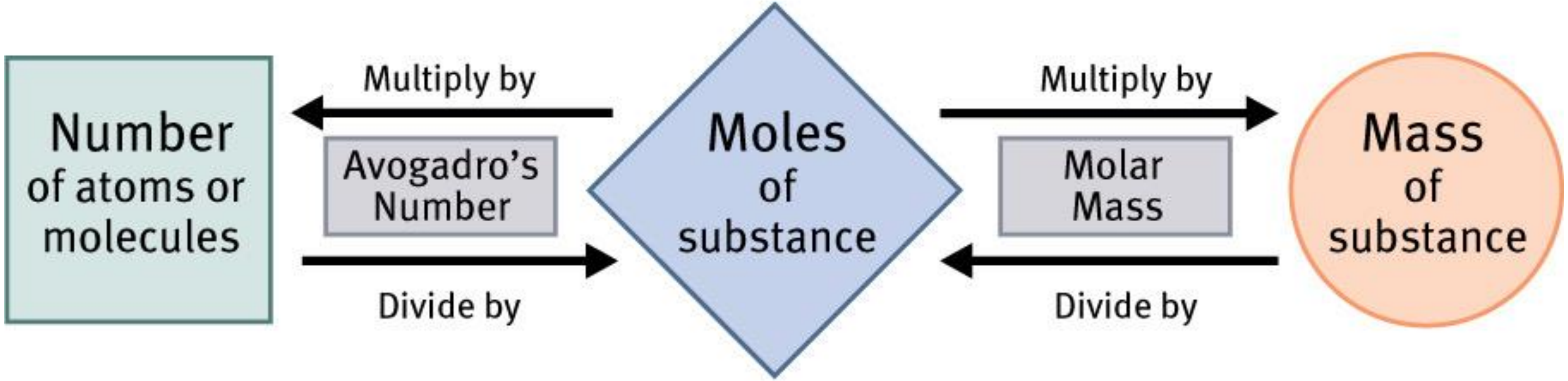
Conversion Between Amount, Mass, and Number

Molar mass and Avogadro's number are essential conversion factors:

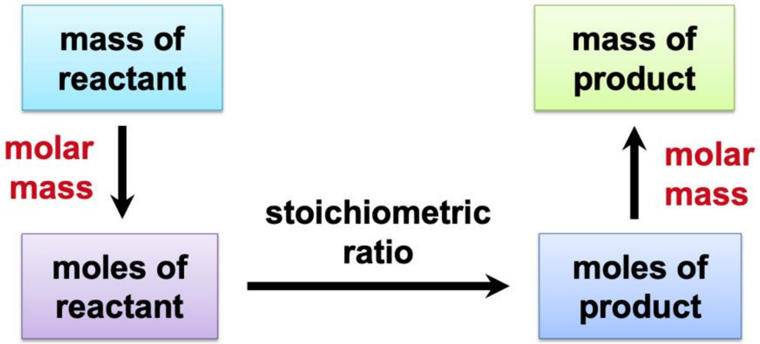


Example of a Mole Method Calculation

Example: If 454 g of NH_4NO_3 decomposes, how much N_2O and H_2O (in grams) are formed?

Step 1: Balanced chemical equation – write out ”givens” and “needs”

Step 2: Calculate moles of “givens”



Step 3: Stoichiometric ratio

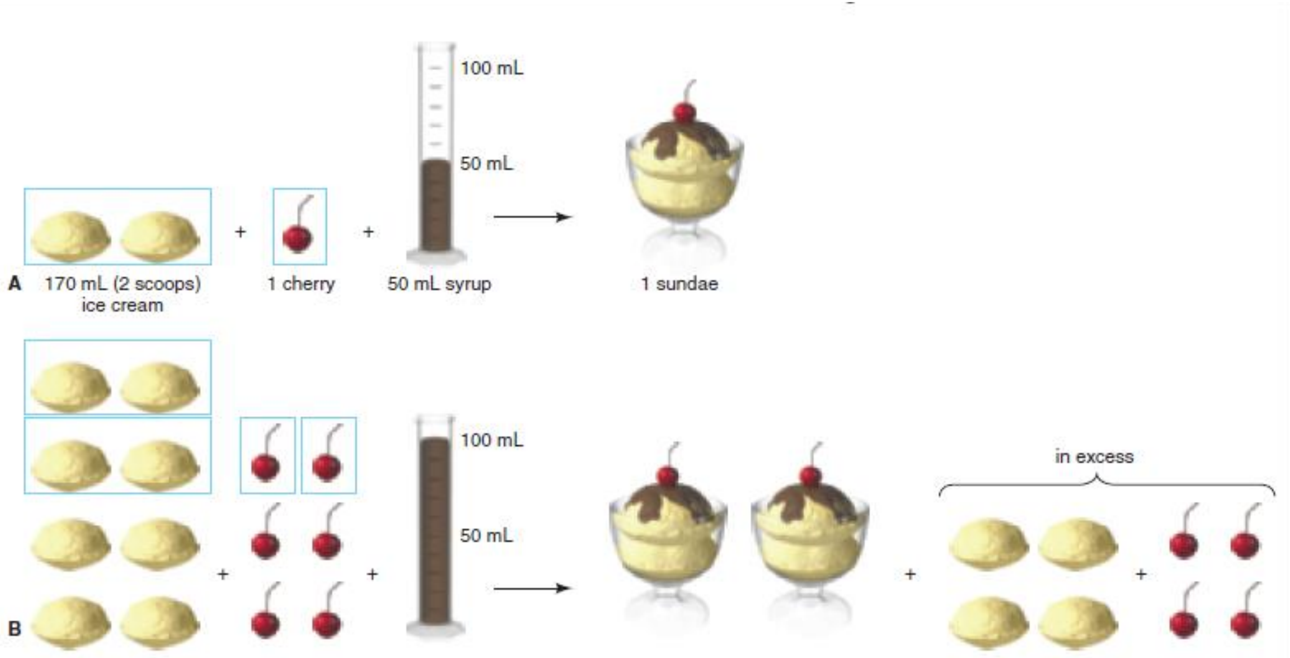
$$n_B = \left(\frac{Coeff_B}{Coeff_A}\right) n_A$$

Stoichiometric ratio

Step 4: Calculate your "needs"

Limiting Reagents

- In real reactions, one reactant can limit the amount of product that can form.
- The limiting reactant will be completely used up in the reaction.
- The reactant that is *not* limiting is in *excess* – some of this reactant will be left over.



Solving Limiting Reactant Problems

1. Write the balanced chemical equation.
2. Convert given quantities into moles.
3. Use reaction stoichiometry to find the amount of product that would be produced by each reagent.
4. The reagent that produces the smallest amount of product is limiting.

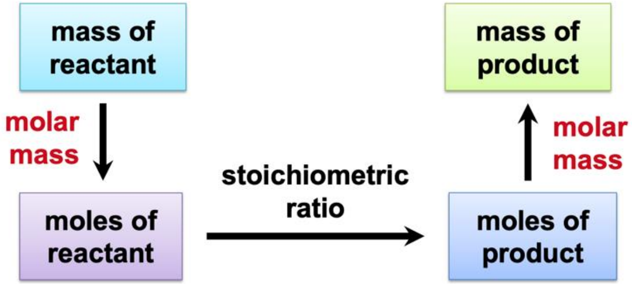
Example: What mass of solid aluminum sulfide can be prepared from the reaction of 10.0 g of aluminum and 15.0 g of sulfur? What mass of the non-limiting reagent is in excess?

Step 1: Write the balanced chemical equation.

Step 2: Convert given quantities into moles.

Step 3: Find the amount of product that would be produced by each given reagent.

Step 4: Calculate the mass of product from the amount of limiting reagent.



Step 5: What mass of the non-limiting reagent is in excess?

Calculate amount required for reaction, and subtract that from amount added to reaction.

Reaction Tables

- Used to keep track of the quantities in a limiting-reactant problem
- Top row shows balanced equation as the column headings.

The table contains rows for reactant and product:

Initial quantities (usually moles)

Change in quantities during the reaction

Final quantities remaining after the reaction

So for the previous example:

$$2\,Al(s) \quad + \quad 3\,S(s) \quad \rightarrow \quad Al_2S_3(s)$$

Initial

Change

Final

Limiting Reactant Example in Solution

Example Problem:

Lead acetate was used as a sweetener before its toxic effects were known. It is possible to distinguish it from sugar by adding it to a NaCl solution, since it will form an insoluble chloride salt.

When 268 mL of 1.50 mol/L lead(II) acetate ($Pb(OAc)_2$) reacts with 130. mL of 3.40 mol/L sodium chloride, what mass (g) of solid lead(II) chloride can form? (Sodium acetate solution also forms.)

Step 1: What is the balanced equation?

Limiting Reactant Example in Solution

Step 2: What is the limiting reagent?

Limiting Reactant Example in Solution

Step 3: Reaction Table

Step 4: Mass of $PbCl_2$ (M = 278.1 g/mol)?

Reaction Yield Calculation

In many reactions, not all the reactants are converted into the desired product. This is calculated using:

$$\text{Percent yield} = 100\% \left(\frac{\text{Actual amount}}{\text{Theoretical amount}} \right)$$

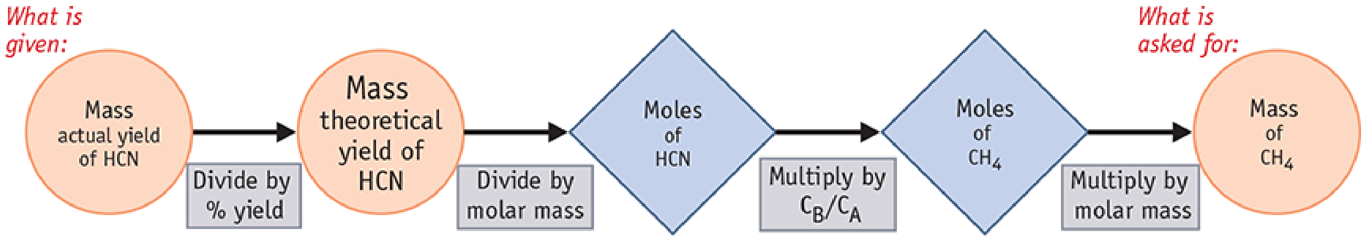
How do we calculate the yield for a multi-step reaction?

e.g. The antidepressant sertraline is synthesized in 6 steps with the following yields: 80%, 80%, 50%, 100%, 48%, and 30%.

Example calculating reactant mass from yield

Example: If the yield of the synthesis of industrial production of hydrogen cyanide is 97.5%, how many kilograms of methane should be used to produce 1.50 x 10^5 kg of HCN?

$CH_4(g) + N_2(g) \rightarrow HCN + H_2(g)$



Step 1: BCE + givens/wants

Example calculating reactant mass from yield

Step 2: Calculate theoretical yield

Step 3: Calculate moles of theoretical yield

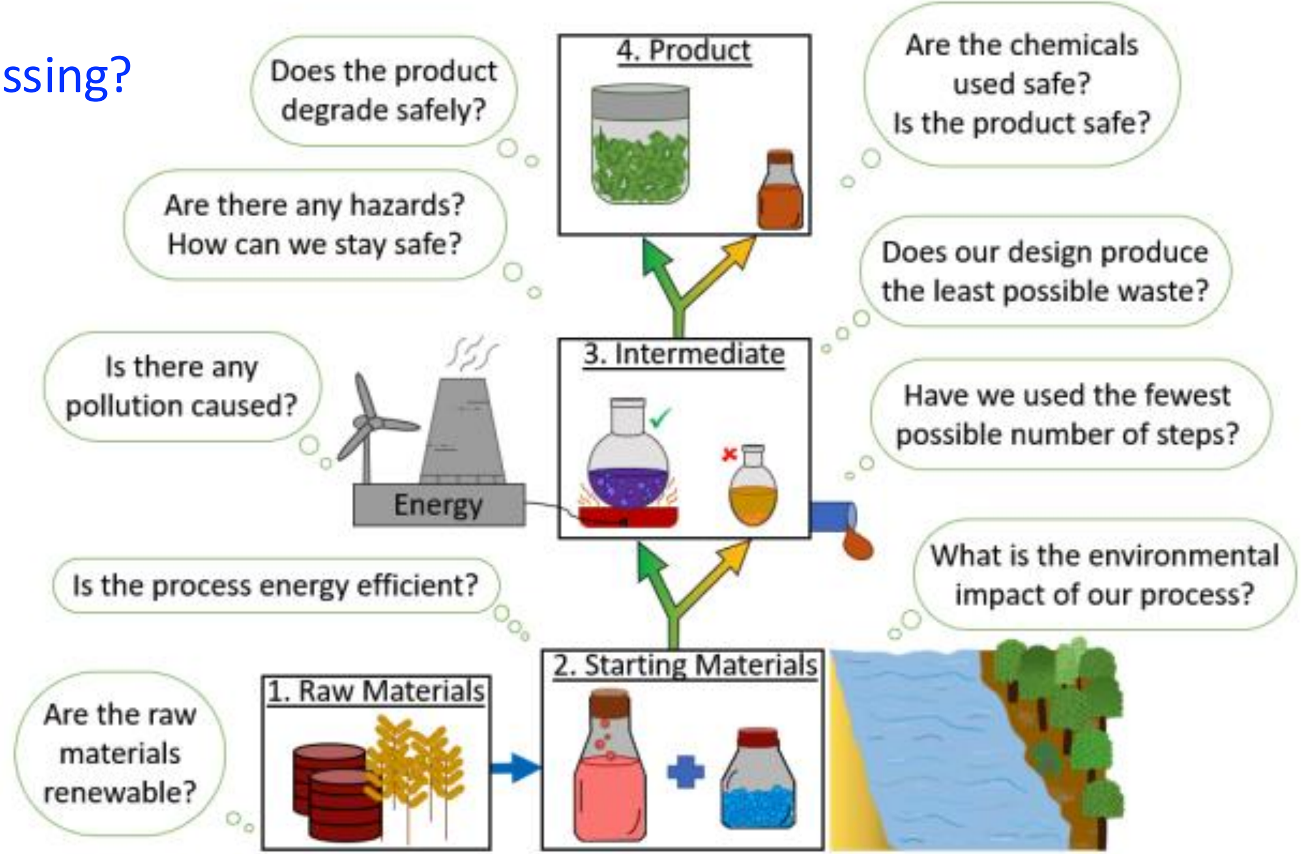
Example calculating reactant mass from yield

Step 4: Use stoichiometric ratio to find moles of CH_4

Step 5: Calculate mass of CH_4

Percent yield has limitations

What is missing?



https://gctlc.org/system/files/2024-01/frontiers-for-young-minds.-green-chemistry-sustainability-at-the-atom-scale.pdf

Established Green Chemistry Metrics

1. Atom economy (atom efficiency)

$$Atom\ Economy\ = \frac{Mass\ of\ desired\ product\ *}{Mass\ of\ all\ reactants*}$$

*including the stoichiometric coefficient

2. Environmental (E) factor

$$E - factor\ = \frac{total\ waste\ (g)}{product\ (g)}$$

Established Green Chemistry Metrics

3. Life Cycle Assessment (LCA)

- An assessment of environmental impacts associated with all of the stages of a product's life.
- Environmental impact of the release of a specified amount of chemical:

$$I = P \, x \, m_{emitted}$$

Impact-based metrics:

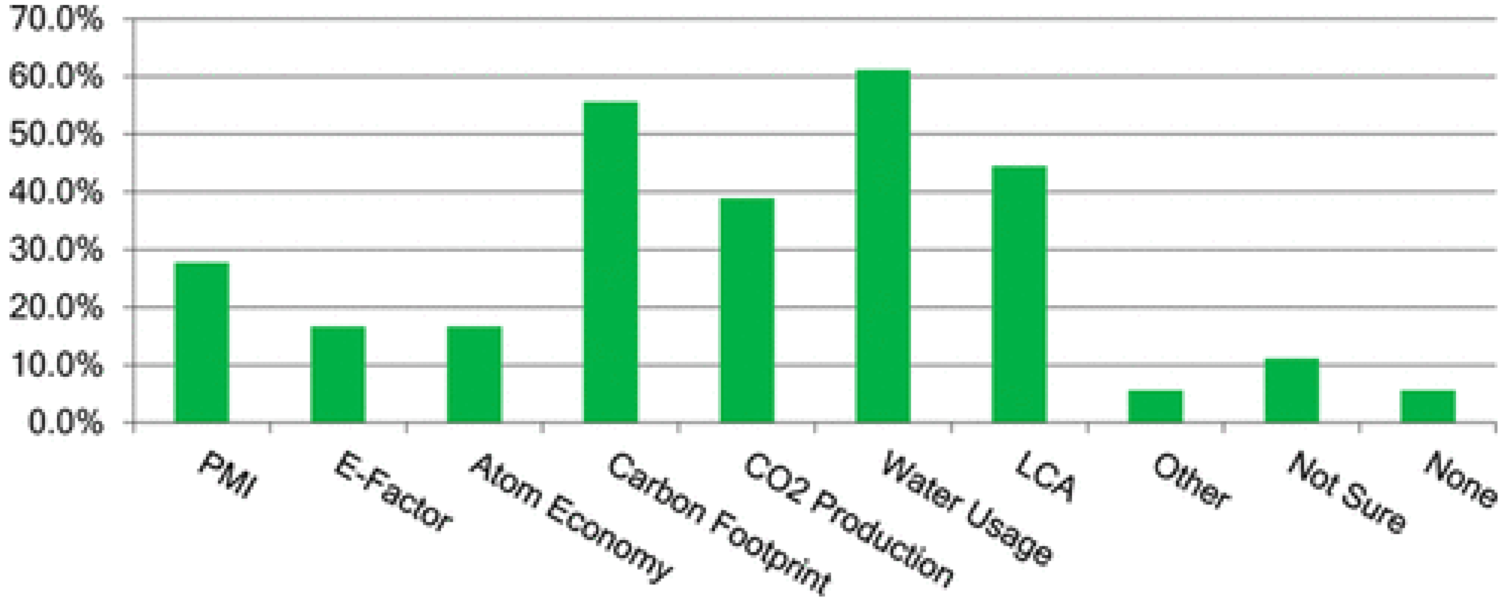
- Global warming
- Smog formation
- Ozone depletion
- Human toxicity
- Eco-toxicity
- Acidification
- Eutrophication

I = impact index
P = impact potential for a substance
m = mass of a substance emitted to the environment, including fugitive emissions or waste

J. Chem. Educ. 2024, 101, 4, 1592–1598

Green Chemistry-Related Metrics used in Chemical Manufacturing

Chemical manufacturer responses (n = 18) to the 2012 Roundtable survey question **"What green chemistry and engineering related metrics does your company use? Select all that apply."**



Implementing Green Chemistry in Chemical Manufacturing: A Survey Report Robert J. Giraud, Paul A. Williams, Amit Sehgal, Ettigounder Ponnusamy, Alan K. Phillips, and Julie B. Manley ACS Sustainable Chemistry & Engineering 2014 2 (10), 2237-2242

Example 1 impact-based metrics: Global warming potential

Example: Garbage decomposing in landfills releases methane gas, which is often “flared” (burned) rather than being vented into the atmosphere. Calculate the global warming caused by releasing 1 mol of methane by venting and by flaring. **Which is less harmful?**

The global warming potentials for CH_4 = 28 and CO_2 = 1,while those of O_2 and H_2O are negligible.

$$CH_4(g) + O_2(g) \rightarrow H_2O(g) + CO_2(g)$$

Natural gas flared vs. vented

Example 2 impact-based metrics: Inhalation toxicity potential

Example: CS_2 is an extremely volatile liquid solvent, boiling at 46 ˚C. It's commonly used to dissolve waste cellulose to make it into fibres called viscose, used in clothing. That takes much less land and water than growing cotton. CS_2 is made by reacting methane (CH_4) with elemental sulfur (S_8) at 600 ˚C. The products are CS_2 and H_2S.

a) Give the balanced reaction equation.
b) If 100 g of methane is reacted with an excess of sulfur, how many grams of CS_2 and H_2S would be produced?
c) Which of those two products, if released into the air, would cause more inhalation toxicity (IINHT)?

Chemical	MW (g/mol)	INHTP (inhalation toxicity potential)
CS_2	76.14	0.84
H_2S	34.08	28.0

Example 2 impact-based metrics: Inhalation toxicity potential

a) Give the balanced reaction equation.

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Example 2 impact-based metrics: Inhalation toxicity potential

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