Measuring the Greenness of Undergraduate Laboratory Experiments

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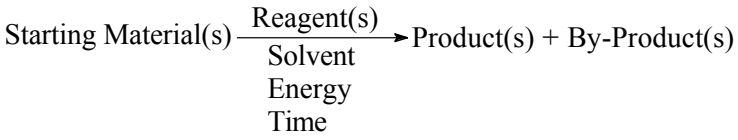
Green vs. Not-Green

- False dichotomy
- Developing one green aspect of an experiment might involve a trade-off with another aspect
- There is really a spectrum of greenness
- Although none is perfect, metrics are available for evaluating greenness

Reaction Components



Familiar Metrics

- Percent yield
- Chemoselectivity
- Regioselectivity
- Enantioselectivity
- Diastereoselectivity
- Mass balance

Metrics for Green Chemistry
("Product-selective Synthesis")

- Percent yield, etc.
- Percentage atom economy, or theoretical atom economy
- Efficiency, or actual atom economy
- Effective mass yield
- Mass productivity
- Others

Atom Economy

$$\frac{\text{MW of Product(s)}}{\text{MW of Starting Material(s) + MW of Reagent(s)}} \times 100$$

Trost, B.M. *Science* **1991**, *254*, 1471-1477.

Percentage Atom Economy (or Theoretical Atom Economy)

$$\frac{\text{FW of Atoms Utilized}}{\text{FW of All Reactants}} \times 100$$

$$\frac{\text{Theoretical Yield of Product(s)}}{\text{Mass of Starting Material(s) + Mass of Reagent(s)}} \times 100$$

Cann, M.C.; Connelly, M.E. *Real-World Cases in Green Chemistry* American Chemical Society: Washington, DC, 2000; pp 5-8.

Efficiency (or Actual Atom Economy)

$$\frac{\text{Actual Yield of Product(s)}}{\text{Mass of Starting Material(s) + Mass of Reagent(s)}} \times 100$$

$$\frac{\text{\% Yield x \% Atom Economy}}{100}$$

Doxsee, K.M.; Hutchison, J.E. *Green Organic Chemistry: Strategies, Tools, and Laboratory Experiments* Brooks/Cole: Belmont, CA, 2004; pp 89-92.

Effective Mass Yield

Effective Mass Yield = Reciprocal of the E-Factor converted to a percentage

What is the E-factor?

E-Factor

$$\frac{\text{Mass of Waste}}{\text{Mass of Product(s)}}$$

$$\frac{\text{Mass of Raw Materials - Mass of Product(s)}}{\text{Mass of Product(s)}}$$

Sheldon, R.A. *CHEMTECH* **1994**, 38-47.

Effective Mass Yield

$$\frac{\text{Mass of Product(s)}}{\text{Mass of Raw Materials - Mass of Product(s)}} \times 100$$

Mass Productivity

$$\frac{\text{Mass of Product(s)}}{\text{Mass of Raw Materials}} \times 100$$

Conclusions

- Metrics are available for evaluating the greenness of a synthesis experiment
- These metrics can be applied to any synthesis experiment
- Green chemistry is a way of thinking about experimental design

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