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

<table>
<thead>
<tr>
<th>Starting Material(s)</th>
<th>Reagent(s)</th>
<th>Solvent</th>
<th>Energy</th>
<th>Time</th>
<th>Product(s)</th>
<th>By-Product(s)</th>
</tr>
</thead>
</table>

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

\[
\text{Atom Economy} = \frac{\text{MW of Product(s)}}{\text{MW of Starting Material(s)} + \text{MW of Reagent(s)}} \times 100
\]


### Percentage Atom Economy

(or Theoretical Atom Economy)

\[
\text{Percentage Atom Economy} = \frac{\text{FW of Atoms Utilized}}{\text{FW of All Reactants}} \times 100
\]

\[
\text{Theoretical Yield of Product(s)} \times \frac{\text{FW of Atoms Utilized}}{\text{FW of All Reactants}} \times 100
\]


### Efficiency

(or Actual Atom Economy)

\[
\text{Efficiency} = \frac{\text{Actual Yield of Product(s)}}{\text{Mass of Starting Material(s)} + \text{Mass of Reagent(s)}} \times 100
\]

\[
\% \text{ Yield} \times \frac{\% \text{ Atom Economy}}{100}
\]

Effective Mass Yield

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

What is the E-factor?

E-Factor

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

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


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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