Implementation of the USEPA’s Waste Reduction Algorithm in Cape-Open Based Process Simulators

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Purpose

• To provide a mechanism to allow environmental and other evaluations of chemical process flowsheets directly from Computer-Aided Process Engineering (CAPE) applications.
Overview

- WAR Algorithm
- Background of the use of CAPE for Environmental Evaluations
- CAPE-OPEN and Flowsheet Monitoring
- Demonstrate WAR using Flowsheet Monitoring
WAR Algorithm

- A one-dimensional sustainability metric – only considers environmental aspects.
- Considers Potential Environmental Impacts (PEI) generated by the process.
- Based on input/output-style balance equations
- Eight impact categories defined in WAR
# WAR IMPACT CATEGORIES

<table>
<thead>
<tr>
<th>General Impact Category</th>
<th>Impact Category</th>
<th>Measure of Impact Category</th>
</tr>
</thead>
<tbody>
<tr>
<td>Human Toxicity</td>
<td>Ingestion</td>
<td>( \text{LD}_{50} )</td>
</tr>
<tr>
<td></td>
<td>Inhalation/Dermal</td>
<td>( \text{OSHA PEL} )</td>
</tr>
<tr>
<td>Ecological Toxicity</td>
<td>Aquatic Toxicity</td>
<td>( \text{Fathead Minnow LC}_{50} )</td>
</tr>
<tr>
<td></td>
<td>Terrestrial Toxicity</td>
<td>( \text{LD}_{50} )</td>
</tr>
<tr>
<td>Global Atmospheric Impacts</td>
<td>Global Warming Potential</td>
<td>( \text{GWP} )</td>
</tr>
<tr>
<td></td>
<td>Ozone Depletion Potential</td>
<td>( \text{ODP} )</td>
</tr>
<tr>
<td>Regional Atmospheric Impacts</td>
<td>Acidification Potential</td>
<td>( \text{AP} )</td>
</tr>
<tr>
<td></td>
<td>Photochemical Oxidation Potential</td>
<td>( \text{PCOP} )</td>
</tr>
</tbody>
</table>
Evolution of WAR

- WAR GUI (Graphical User Interface): Outside of simulation package, manual user input.
- WAR In Aspen (Fu et al. 2000) Also implemented optimization blocks.
- Implemented in ChemCAD and ICAS: One-off private implementations.
- CO-WAR (Fermaglia et al. 2008): Used CAPE-OPEN unit operation placed in each stream of interest to get stream data.
- What is missing is a single, multi-package implementation.
Flowsheet Monitoring

- Allows access to simulation data for applications that require
  - Access to multiple parts of the flowsheet
  - Thermodynamic models,
- Does not interfere with the flowsheet itself.
- Flowsheet monitoring applications generally perform post-processing on flowsheet calculations, such as flowsheet evaluation and validation.
WAR With Flowsheet Monitoring

- USE Flowsheet monitoring interfaces in COFE
- Obtains flowsheet monitoring object from the simulation context.
- Obtains unit operation and material stream collection from the flowsheet monitoring object.
- Identifies input and output streams using unit operations and their ports.
- Obtains material and energy flows directly from the streams.
- Uses flow data to calculate WAR PEI values.
DEMONSTRATION
Concluding Remarks

• Prototype flowsheet monitoring interfaces have been implemented in COFE.
• Currently under development by the Method and Tools SIG.