HIGH PRODUCTION VOLUME CHEMICALS –

UNDERSTANDING THE GREEN CHEMISTRY & POLLUTION PREVENTION IMPLICATIONS

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Professor Michael Overcash
Department of Chemical and Biomolecular Engineering
North Carolina State University

Perspective on the Universe of Chemicals in Commerce

- General definition - >1mt/yr in production
- Origin is the New Source Registration Program at USEPA, FDA, and US Dept. of Agriculture

- ~ 100,000 chemicals

- Of which ~ 30,000 are polymers
  - ~ 10,000 are drug-related (FDA)
  - ~ 10,000 are agricultural chemicals (USDA)
- Grows at about 1%/year

Commodity Chemicals

- Designation in the Chemical Industry for the high product volume in commerce

- Usually these are 50 in number

  – 60% are organics (in the range or 1.5 – 15 million metric tons per year)

  – 40% are inorganics (larger: in the range of 1-45 million metric tons per year)

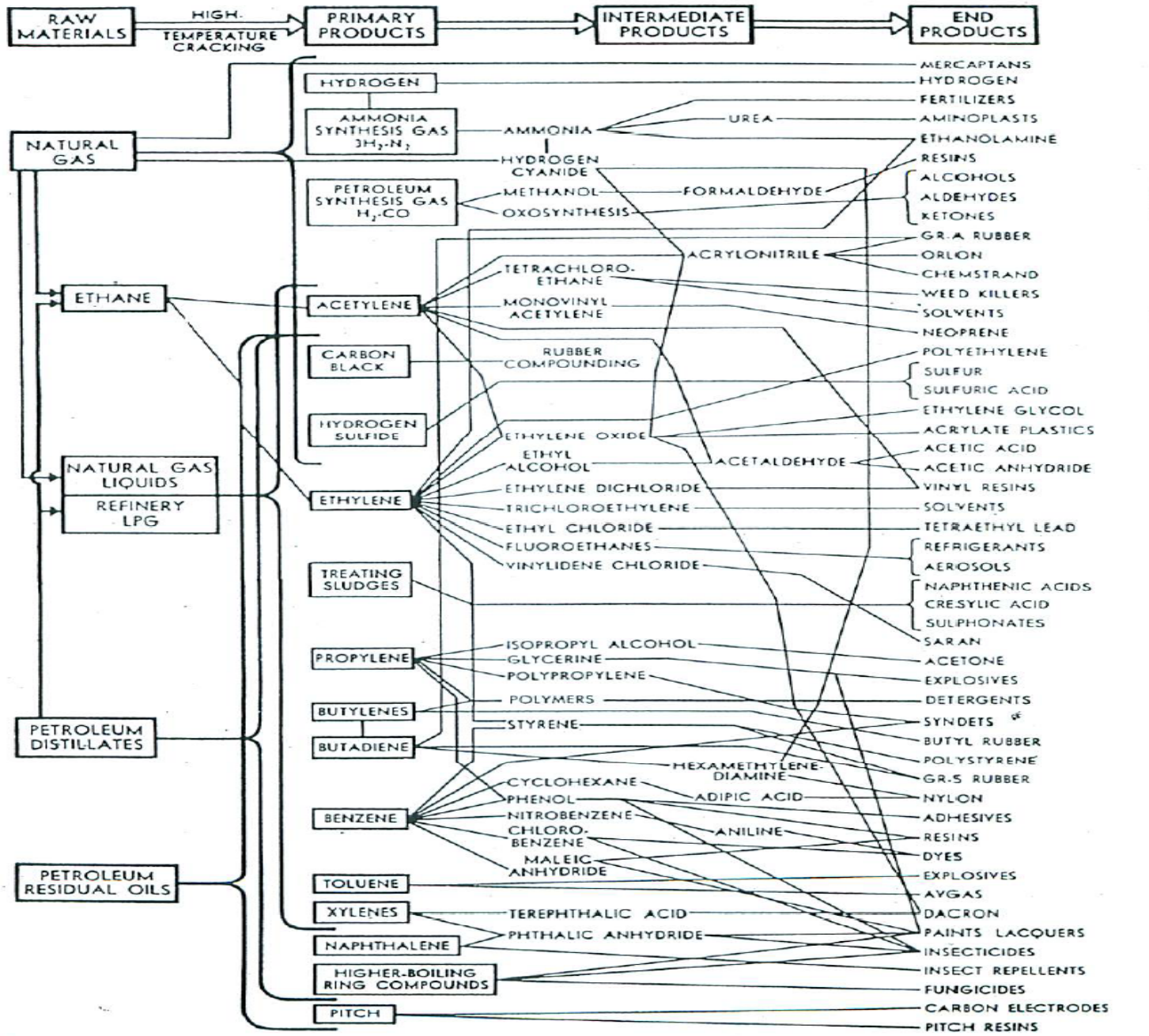


FIG. 20-1. Some of the petrochemicals that can be produced from natural gas, natural-gas liquids, and petroleum. (*Pet. Refiner.*)

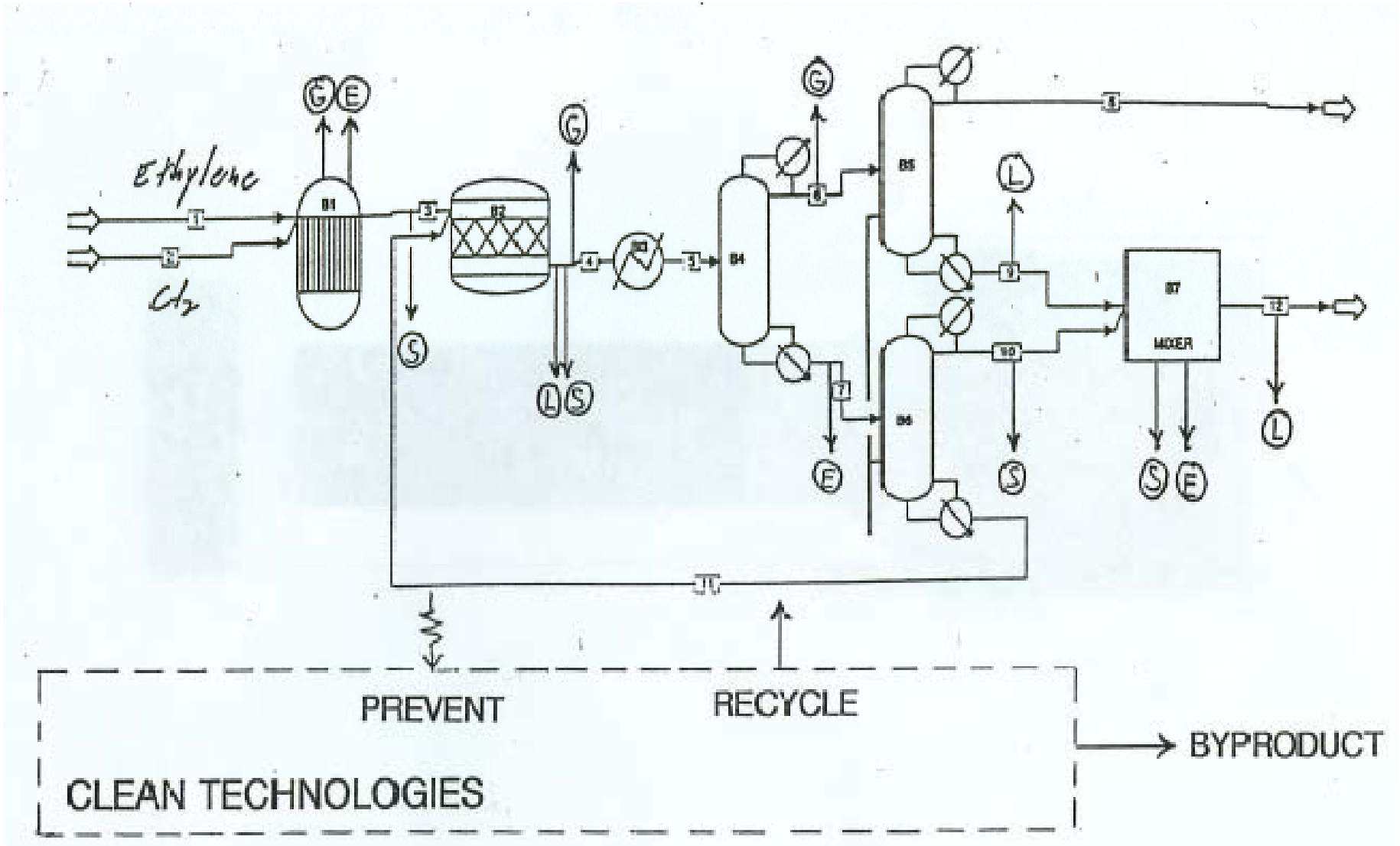
High Production Volume Chemicals

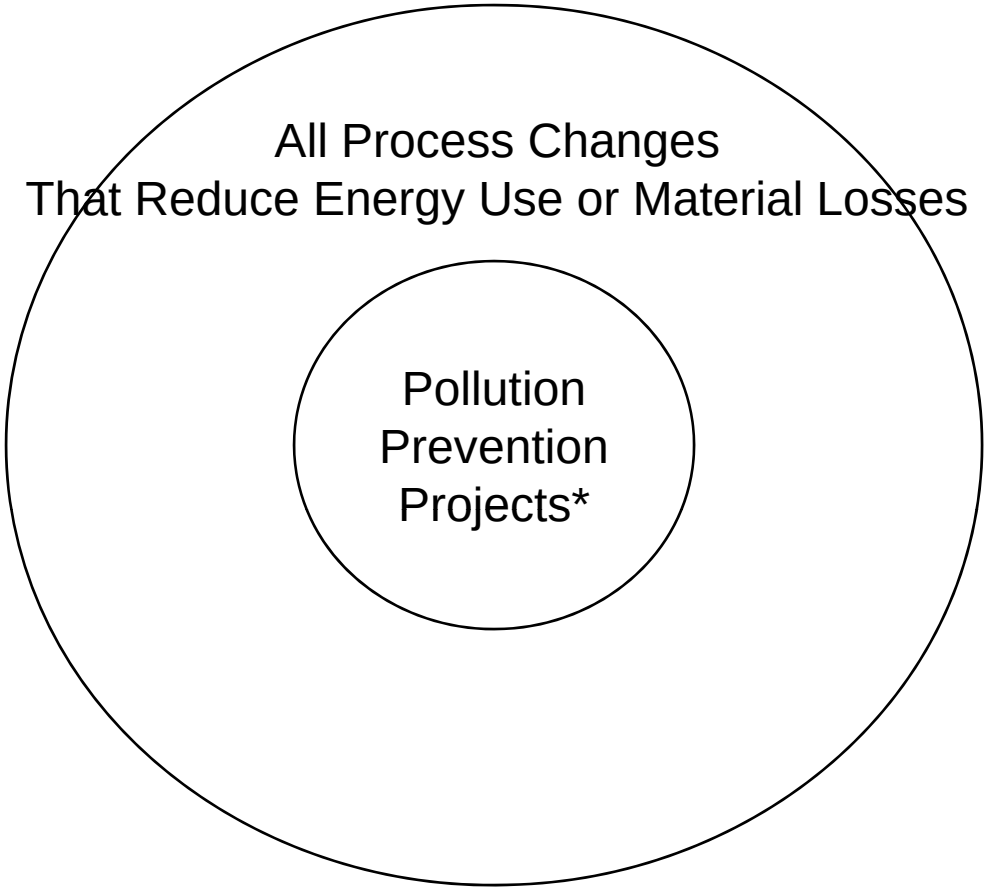
- About 2,500 chemicals (threshold about 12 mt/yr)
- Appear to be almost all organics
- Not yet developed correlations with other lists used in industry or in research for green chemistry & pollution prevention

HPV Future Challenges

- After the assembly and verification of the HPV database
- Challenge shifts to environmental improvement
- Goal is to stimulate changes in manufacturing and products that reduce adverse effects of HPVs
- Green chemistry and pollution prevention will likely play a significant role
- Life cycle thinking will be necessary to achieve net improvement

Perspective on Pollution Prevention


Ethylene
Cl2
MIXER
PREVENT
RECYCLE
BYPRODUCT
CLEAN TECHNOLOGIES



* Cost-Effective Changes

Context of Pollution Prevention Within All Possible Process Changes

Sources of P2 Case Studies

- Pollution Prevention Library of Case Studies (North Carolina Office of Waste Reduction) – About 41,000 On-line Papers or Reports (2007)

  – http://www.P2PAYS.org

Green Chemistry and Pollution Prevention - Observations

- Green chemistry is a newer focus to enable renewed effort in industry (list of principles)

- Green chemistry is primarily viewed in relation to chemical manufacturing, while P2 is both chemical and product manufacturing

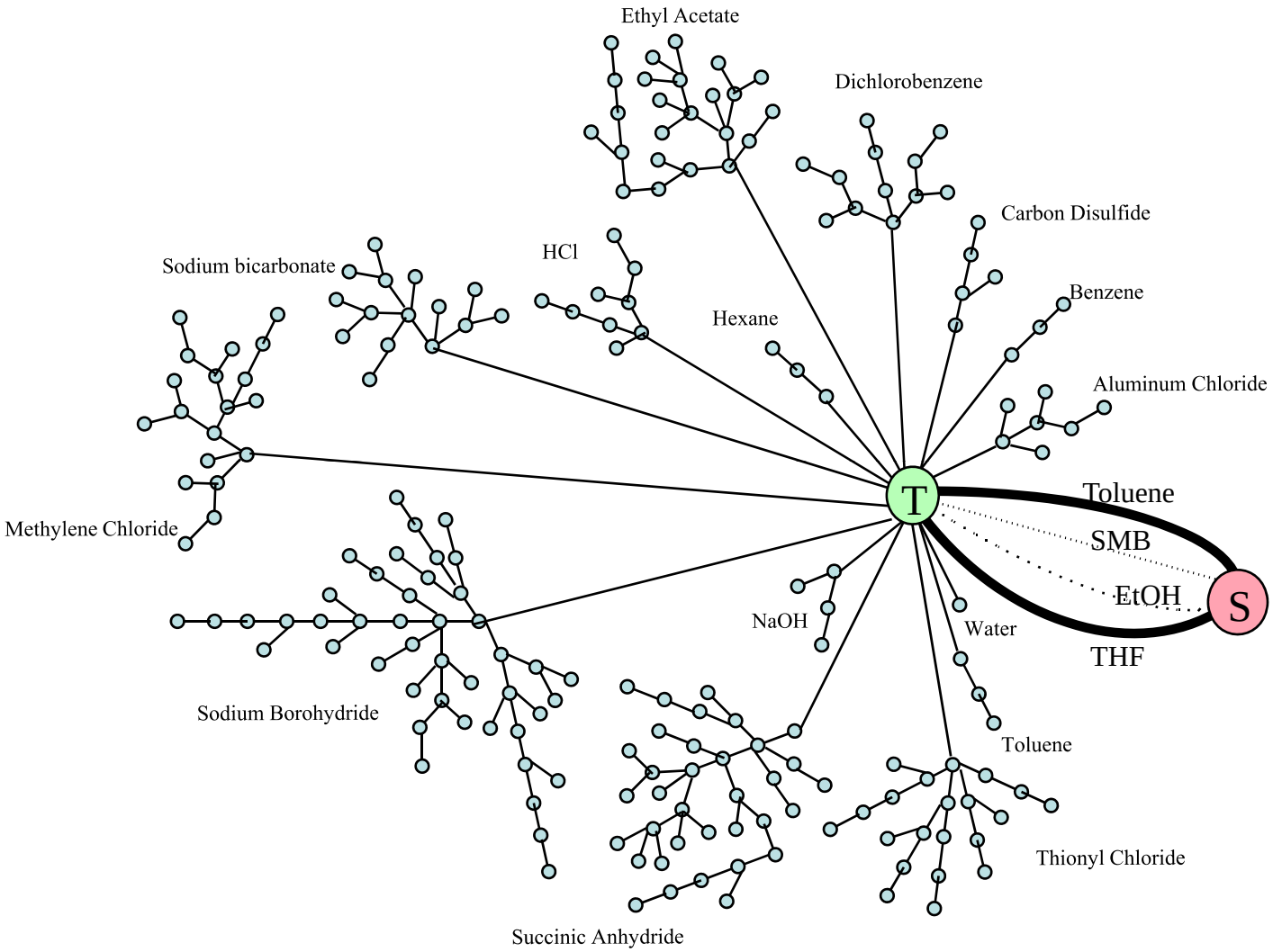
- Green chemistry has not made explicit the economic payback requirements for implementation

Green Chemistry Principles (12)

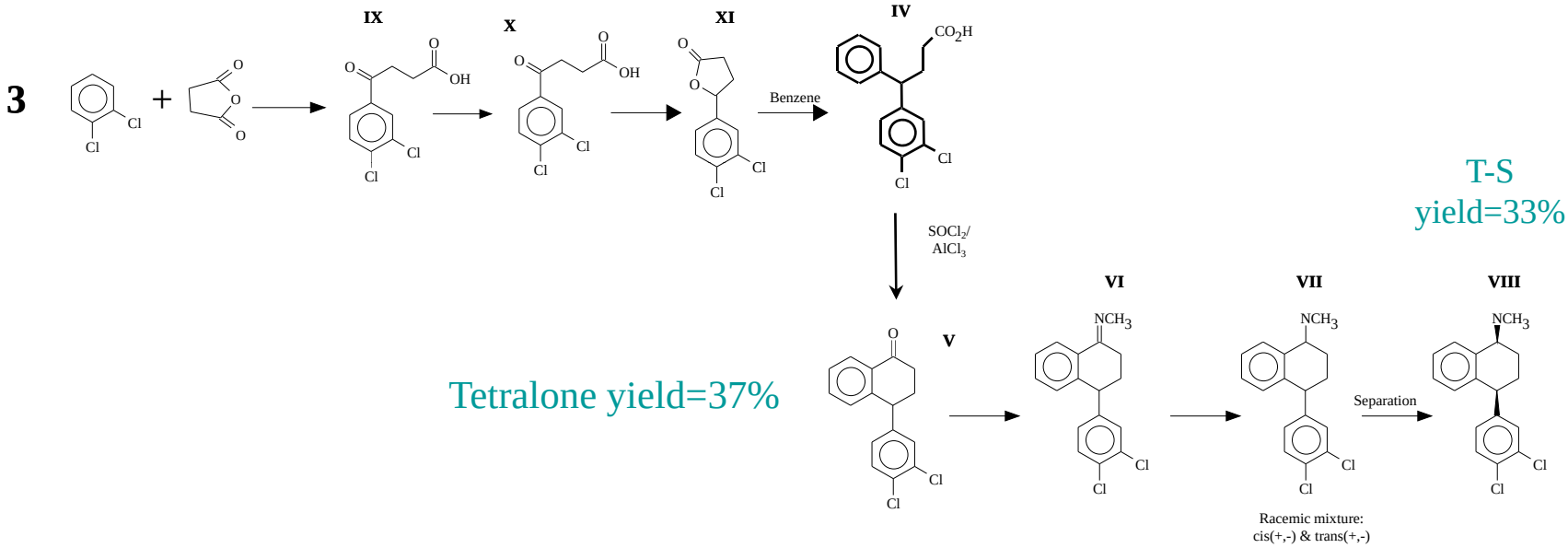
1. Non hazardous inputs and outputs
2. Prevent first
3. Minimize separation energy
4. Maximize energy and mass efficiency
5. Focus on output need
6. Embedded entropy influences reuse
7. Durability not immortality

Continued

8. Unnecessary capacity is a design flaw
9. Minimize material and component diversity
10. Product integration with energy and materials flows
11. Preference for reuse at end-of-life
12. Use renewables


Ethyl Acetate
Dichlorobenzene
Carbon Disulfide
Benzene
Aluminum Chloride
Toluene
SMB
EtOH
THF
S
T
Water
Toluene
Thionyl Chloride
NaOH
Succinic Anhydride
Sodium Borohydride
Methylene Chloride
Sodium bicarbonate
HCl
Hexane

“Carbon frame” efficiency



T-S
yield=33%

Tetralone yield=37%

Total yield=12.2%

10% IMPROVEMENT IN CARBON UTILIZATION EFFICIENCY

- **WITHIN THE COMPANY (kg/kg Sertraline):**

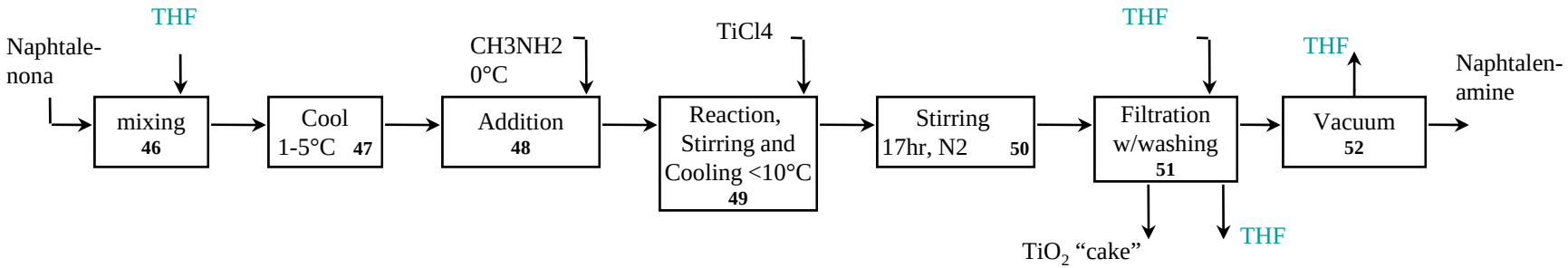
  97 ⇨ **96** ⟷ **1 (most waste is solvent)**

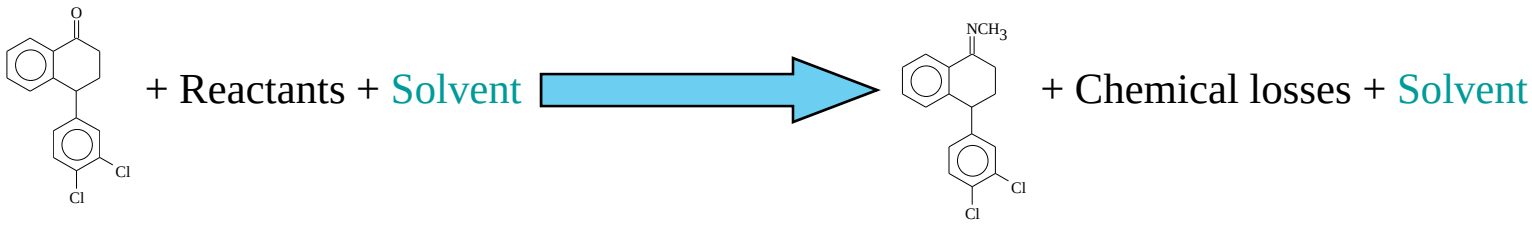
- **THROUGHOUT THE PHARMACEUTICAL COMPLEX (kg/kg Sertraline)**

  39,098 ⇨ **35,794** ⟷ **3,304**

Over 3,000-fold greater impact

Solvent usage efficiency





10% IMPROVEMENT INSOLVENT USAGE

- WITHIN THE COMPANY (kg/kg Sertraline)

97 ⇨ 89 ⟷ 8

- WITHIN THE PHARMACEUTICAL COMPLEX (kg/kg Sertraline)

39,098 ⇨ 38,493 ⟷ 605

LARGER EFFECT WITHIN COMPANY,
BUT GREATEST IMPACT IS OUTSIDE COMPANY

P2 Solutions

- Recycle – increases yield and reduces the entire supply chain, which can include additional HPVs

- Prevention – substitution leads to introduction of a new segment of the supply chain and increase HPVs

  - increased yield and reduces the entire supply chain, which can include HPVs

- Reuse as byproduct
  - eliminates the production of the reused HPV material
  - may also reduce more HPVs in the supply chain avoided

Future Work: Begin Thinking about the HPV Program Decision-making

- Perform an example of green chemistry solutions with life cycle information for 1-4 HPV chemicals to help those working on improvement to see some of the hidden benefits of change.

- Examine the human health assessment (DALY's) from the supply chain versus the use of an HPV chemical to see the relative importance of information.

Conclusions

1. HPV and other chemicals are a part of the large scale societal use of “chemicals in commerce”

2. Environmental improvements for HPVs from green chemistry & pollution prevention must also be reviewed in terms of the life cycle effects on human health and the environment

3. A challenge is to make the HPV lists more useable and searchable in the techniques used for Green Chemistry & P2