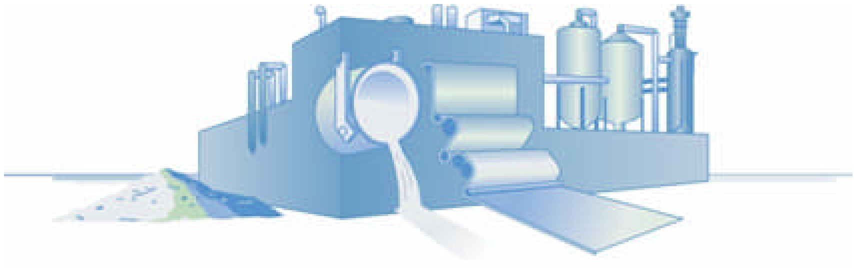
U.S. Department of Energy
Energy Efficiency and Renewable Energy

industrial technologies program

ITP Chemicals Bandwidth Study



Dr. Dickson Ozokwelu
US Department of Energy
Office of Energy Efficiency and Renewable Energy
Industrial Technologies Program
December 6, 2006

Contributors

- Dr. Dickson Ozokwelu, *DOE-ITP*
- Dr. Joseph Rogers, *AIChE*
- Dr. Joseph Porcelli, *JVP, Inc.*
- Dr. Peter Akinjiola, *Psage Research*
- Dr. Juergen Hahn, *Texas A&M University*
- Melanie Miller, *Energetics*
- Karla Bell, *BCS, Inc.*

Outline of Presentation

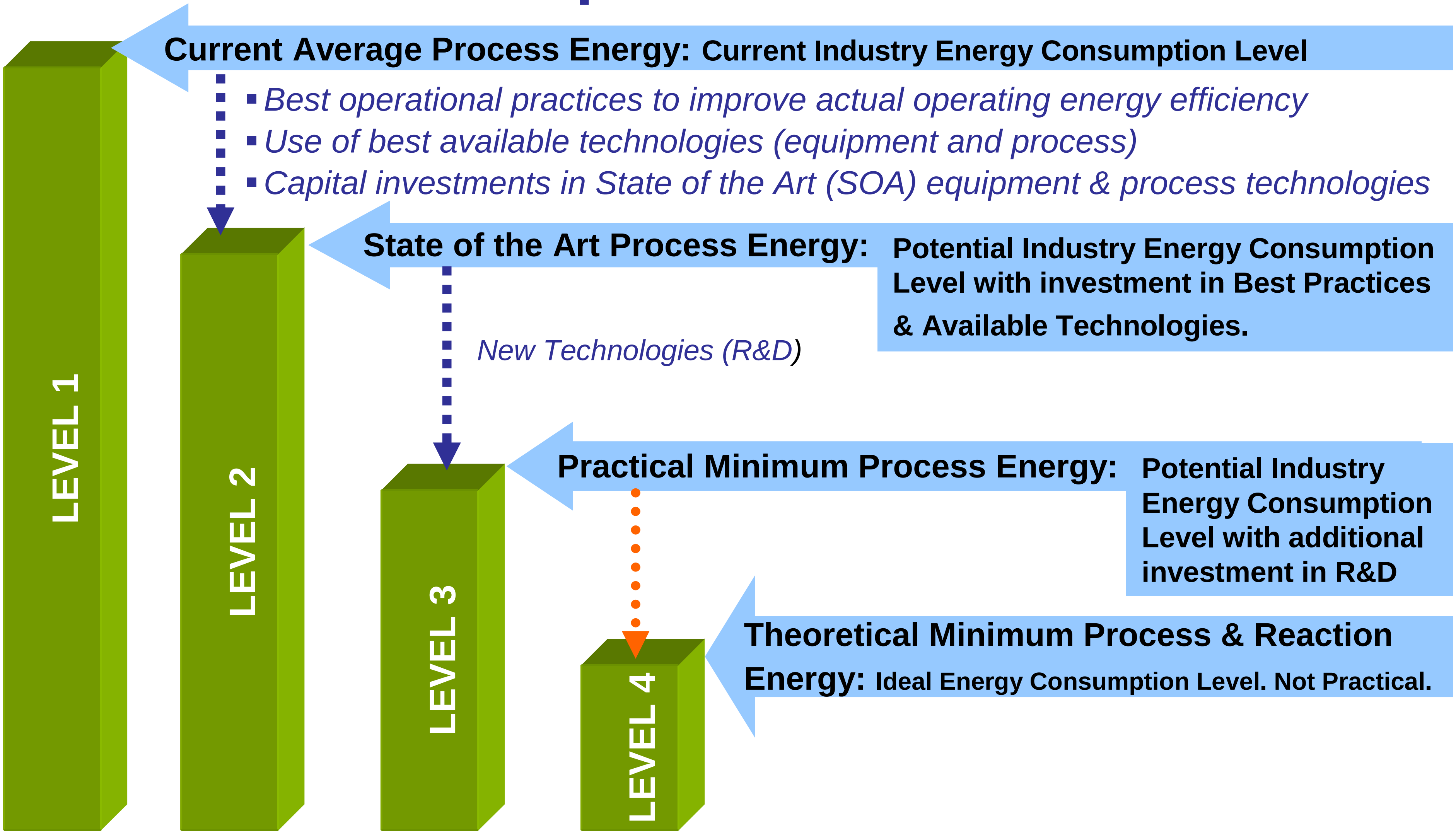
- What is bandwidth? – Basic definitions
- Why do bandwidth study? – Purpose
- What was done?
- How it was done?
- Findings and trends
- Questions and Answers
- Visit DOE-EERE-ITP Chemicals Website for full report

What is Energy Bandwidth Analysis?

Energy bandwidth analysis provides a measure of opportunities for energy savings through improvements in technology, process design, operating practices, or other factors. Bandwidth analysis quantifies the differences between plant process energy consumption levels. (See next slide)

1. **Current average process energy**
2. **State of the art process energy**
3. **Practical minimum process energy**
4. **Theoretical minimum energy**
    a. **Theoretical minimum p*rocess* energy**
    b. **Theoretical minimum r*eaction* energy**

Bandwidth Descriptions



Current Average Process Energy: **Current Industry Energy Consumption Level**

- *Best operational practices to improve actual operating energy efficiency*
- *Use of best available technologies (equipment and process)*
- *Capital investments in State of the Art (SOA) equipment & process technologies*

State of the Art Process Energy: **Potential Industry Energy Consumption Level with investment in Best Practices & Available Technologies.**

New Technologies (R&D)

Practical Minimum Process Energy: **Potential Industry Energy Consumption Level with additional investment in R&D**

Theoretical Minimum Process & Reaction Energy: **Ideal Energy Consumption Level. Not Practical.**

Why was it done?

- To better focus our portfolio to support ITP mission and goals
- To guide research decision-making and ensure that Federal funds are spent effectively.
- Identify top energy/exergy-consuming technology areas at the unit operation level: reactions, distillation, extraction, drying, etc
- Exergy analysis can pinpoint areas within process responsible for major recoverable energy losses
- Focus responses to solicitations on areas that can make greatest impact

The Industrial Technologies Program (ITP)

Mission: Reduce the energy intensity of U.S. industry through coordinated R&D, validation, and dissemination of innovative technologies and practices.

Partnerships

Collaborative R&D

- Energy-intensive Process Technologies
- Crosscutting Technologies

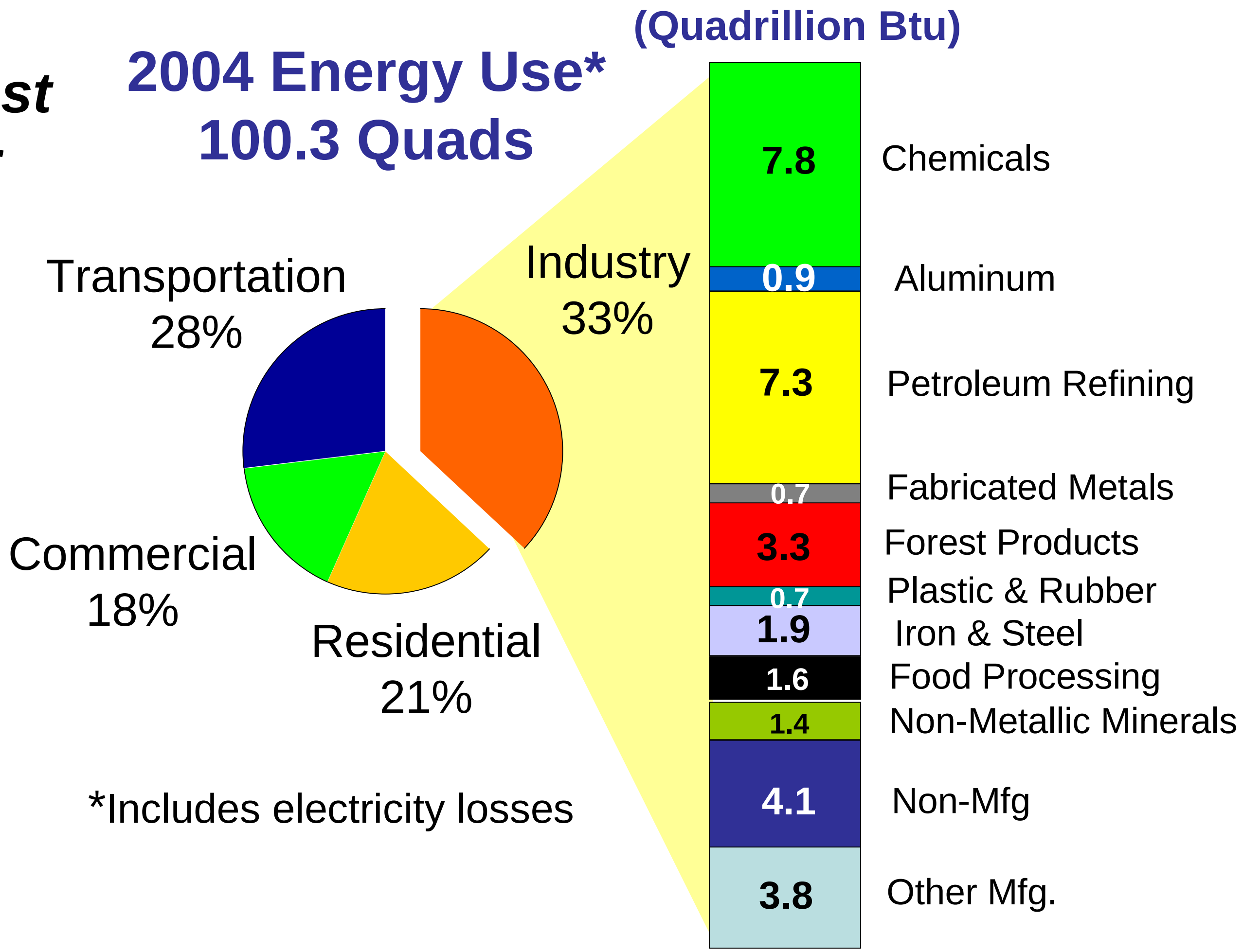
Technology Delivery

- Assessments
- Training & Tools
- Technology Demonstrations

Focus on Energy-Intensive Industries

Industry is the largest energy using sector

- 37% of U.S. natural gas demand
- 29% of U.S. electricity demand
- 30% of U.S. greenhouse gas emissions

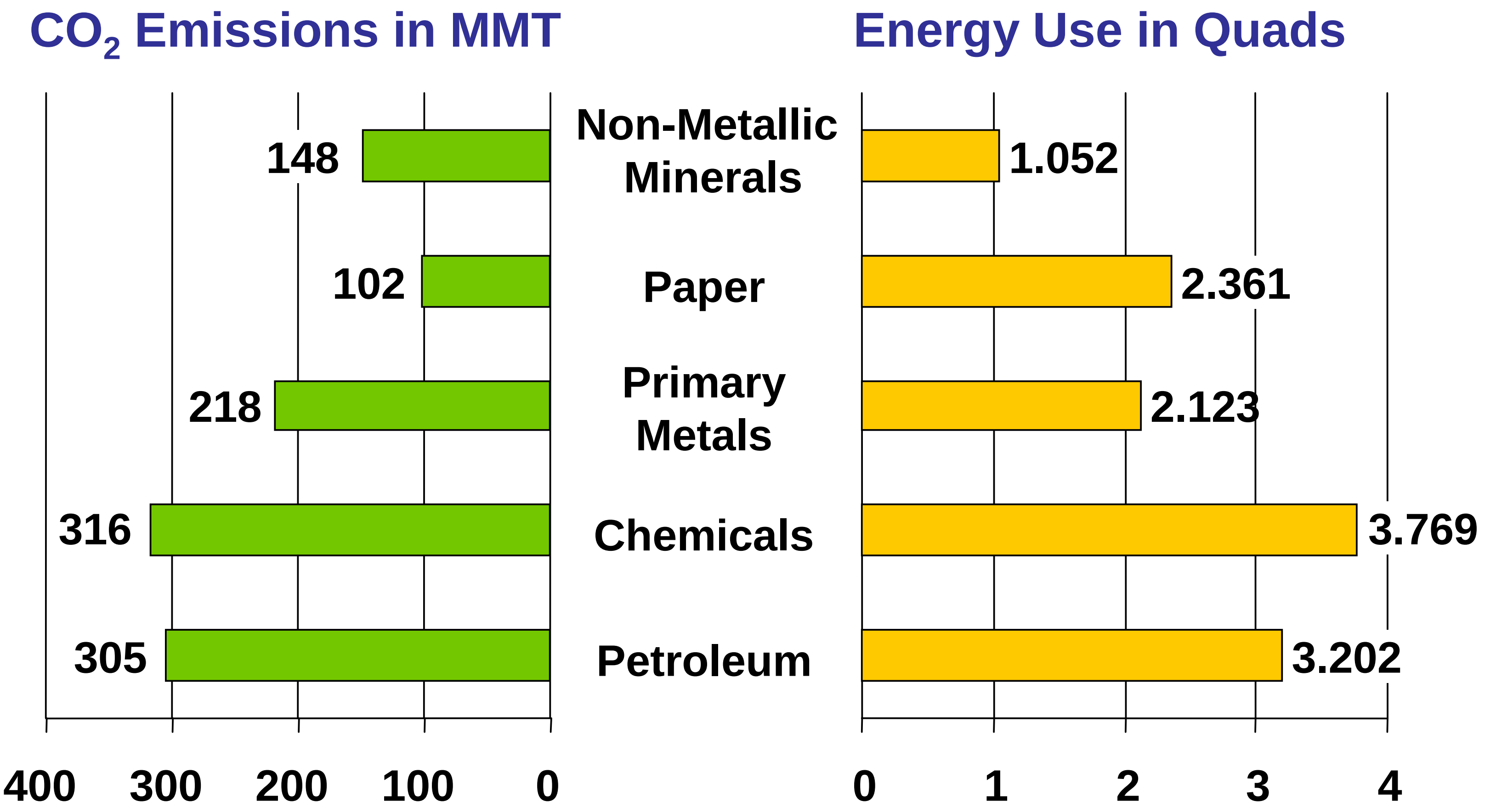


2004 Energy Use*
100.3 Quads

*Includes electricity losses

Source: DOE/EIA Monthly Energy Review 2004 (preliminary) and estimates extrapolated from MECS

CO$_2$ Emissions Relative to Energy Use



U.S. Manufacturing = 1,471 MMT

U.S. Manufacturing = 16.276 quads

What was done?

- **Studied 53 process technologies for production of 44 major chemical products**
  - **Among largest volume chemicals**
  - **Among highest Energy consumers**

- **For each process and for each type of equipment**
  - **Analyzed reasons for high Energy/Exergy losses**
  - **Recommended areas of future research**

How was it done?

- Chose process technologies to be studied
- Model the process technology
  - Aspen Tech – AspenPlus 11.1 version
  - AspenPEP library – A database of SRI process models built into AspenPlus Flowsheet models
  - Open literature – Data to support detailed steady-state process model
- Perform energy and exergy analysis
  - Energy/exergy of each stream – ExerCom (Jacobs Engineering)
  - Energy/exergy of each process unit – Psage-developed software
- Interpret results

Chemicals Selected for Analysis

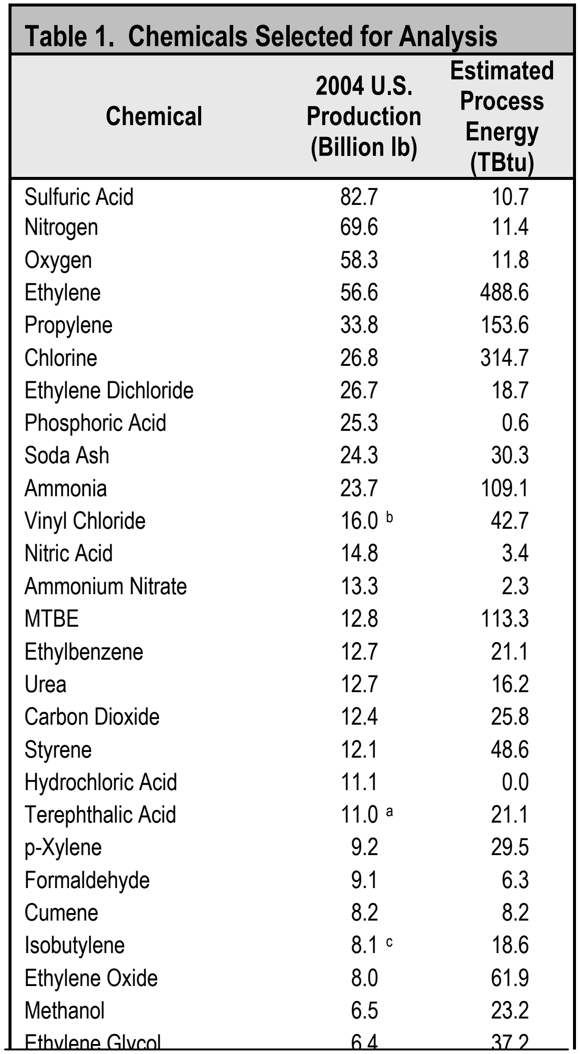


Table 1. Chemicals Selected for Analysis

Chemical	2004 U.S. Production (Billion lb)	Estimated Process Energy (TBtu)
Sulfuric Acid	82.7	10.7
Nitrogen	69.6	11.4
Oxygen	58.3	11.8
Ethylene	56.6	488.6
Propylene	33.8	153.6
Chlorine	26.8	314.7
Ethylene Dichloride	26.7	18.7
Phosphoric Acid	25.3	0.6
Soda Ash	24.3	30.3
Ammonia	23.7	109.1
Vinyl Chloride	16.0 [b]	42.7
Nitric Acid	14.8	3.4
Ammonium Nitrate	13.3	2.3
MTBE	12.8	113.3
Ethylbenzene	12.7	21.1
Urea	12.7	16.2
Carbon Dioxide	12.4	25.8
Styrene	12.1	48.6
Hydrochloric Acid	11.1	0.0
Terephthalic Acid	11.0 [a]	21.1
p-Xylene	9.2	29.5
Formaldehyde	9.1	6.3
Cumene	8.2	8.2
Isobutylene	8.1 [c]	18.6
Ethylene Oxide	8.0	61.9
Methanol	6.5	23.2
Ethylene Glycol	6.4	37.2

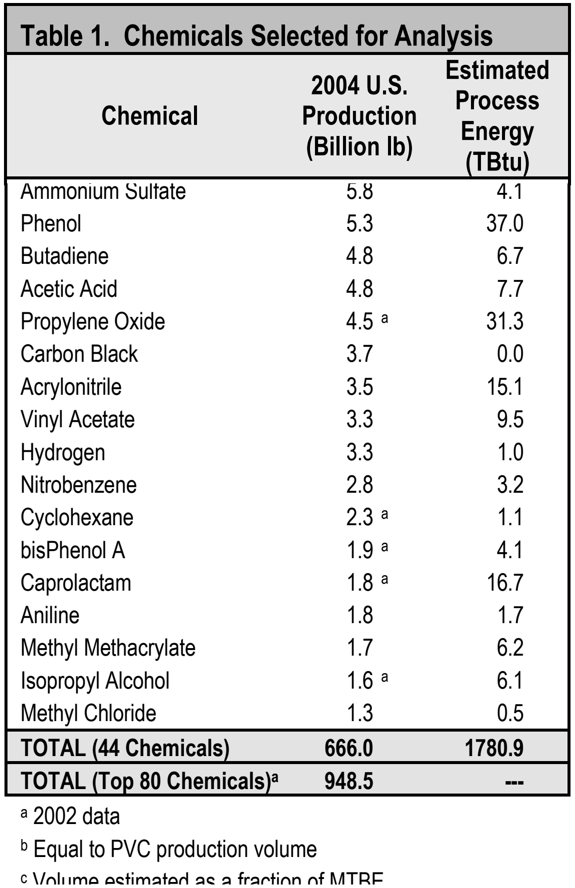


Table 1. Chemicals Selected for Analysis

Chemical	2004 U.S. Production (Billion lb)	Estimated Process Energy (TBtu)
Ammonium Sulfate	5.8	4.1
Phenol	5.3	37.0
Butadiene	4.8	6.7
Acetic Acid	4.8	7.7
Propylene Oxide	4.5 [a]	31.3
Carbon Black	3.7	0.0
Acrylonitrile	3.5	15.1
Vinyl Acetate	3.3	9.5
Hydrogen	3.3	1.0
Nitrobenzene	2.8	3.2
Cyclohexane	2.3 [a]	1.1
bisPhenol A	1.9 [a]	4.1
Caprolactam	1.8 [a]	16.7
Aniline	1.8	1.7
Methyl Methacrylate	1.7	6.2
Isopropyl Alcohol	1.6 [a]	6.1
Methyl Chloride	1.3	0.5
TOTAL (44 Chemicals)	**666.0**	**1780.9**
TOTAL (Top 80 Chemicals)[a]	**948.5**	**---**

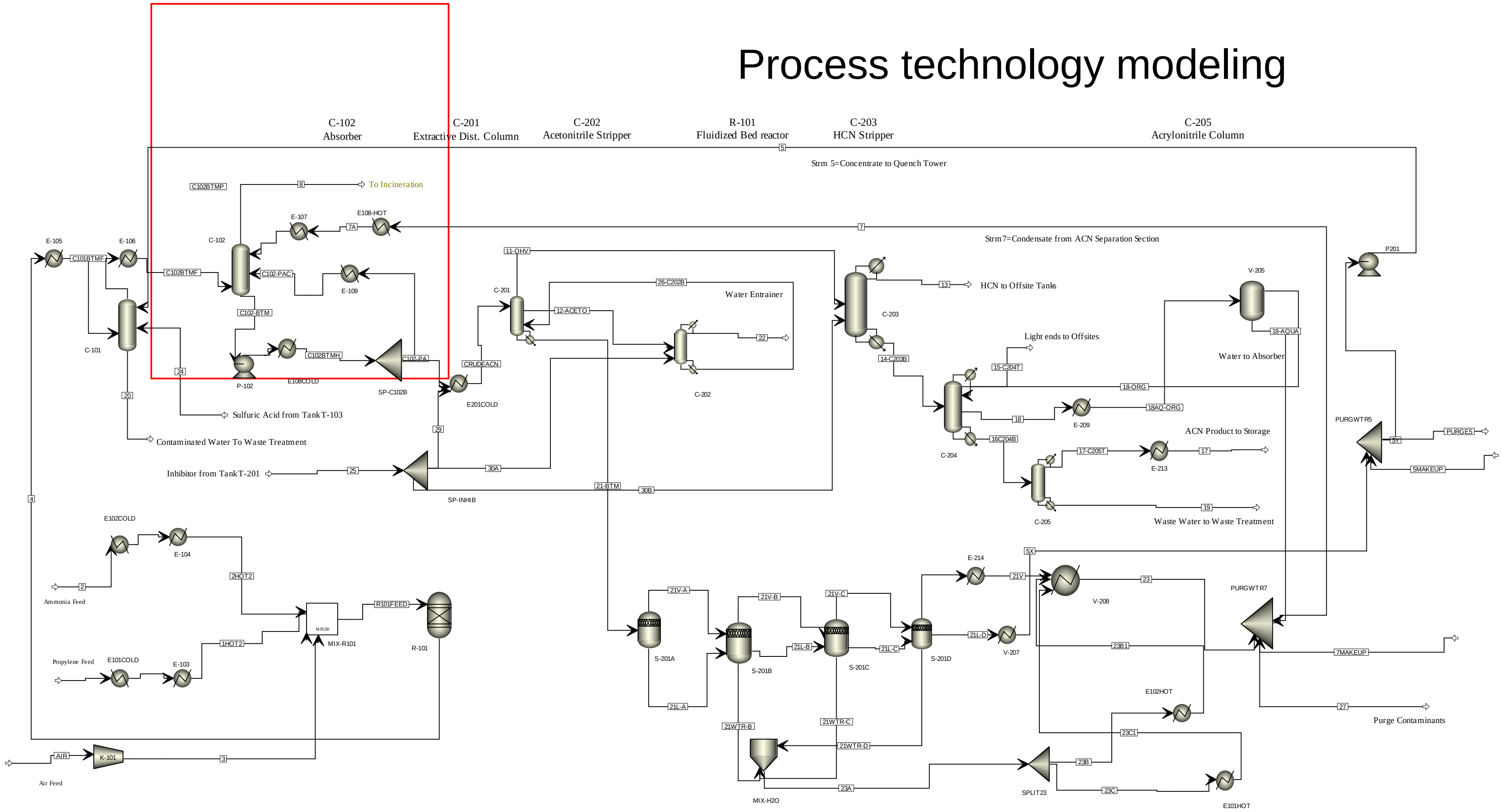
[a] 2002 data

[b] Equal to PVC production volume

[c] Volume estimated as a fraction of MTBE

How was it done?

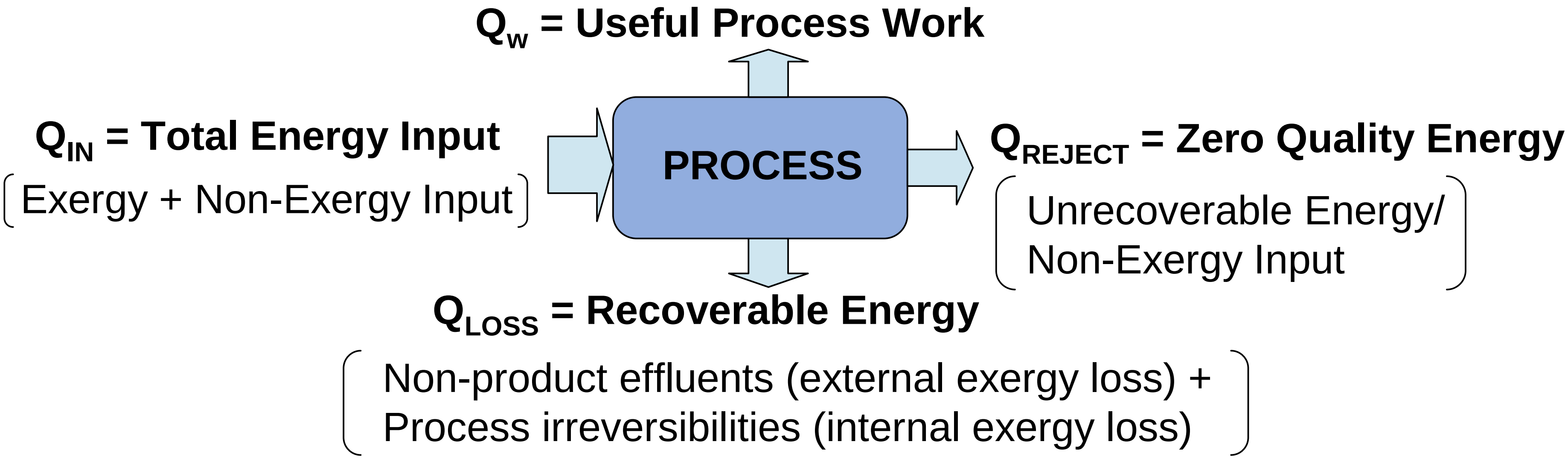
Process technology modeling



AspenPlus Flowsheet Model: Acrylonitrile from Propylene Ammoxidation Process (SOHIO)

How it was done? --- Exergy Analysis

$$Q_{IN} = Q_{W} + Q_{LOSS} + Q_{REJECT}$$



Q_w = Useful Process Work

Q_{IN} = Total Energy Input

Exergy + Non-Exergy Input

Q_{REJECT} = Zero Quality Energy

Unrecoverable Energy/
Non-Exergy Input

Q_{LOSS} = Recoverable Energy

Non-product effluents (external exergy loss) +
Process irreversibilities (internal exergy loss)

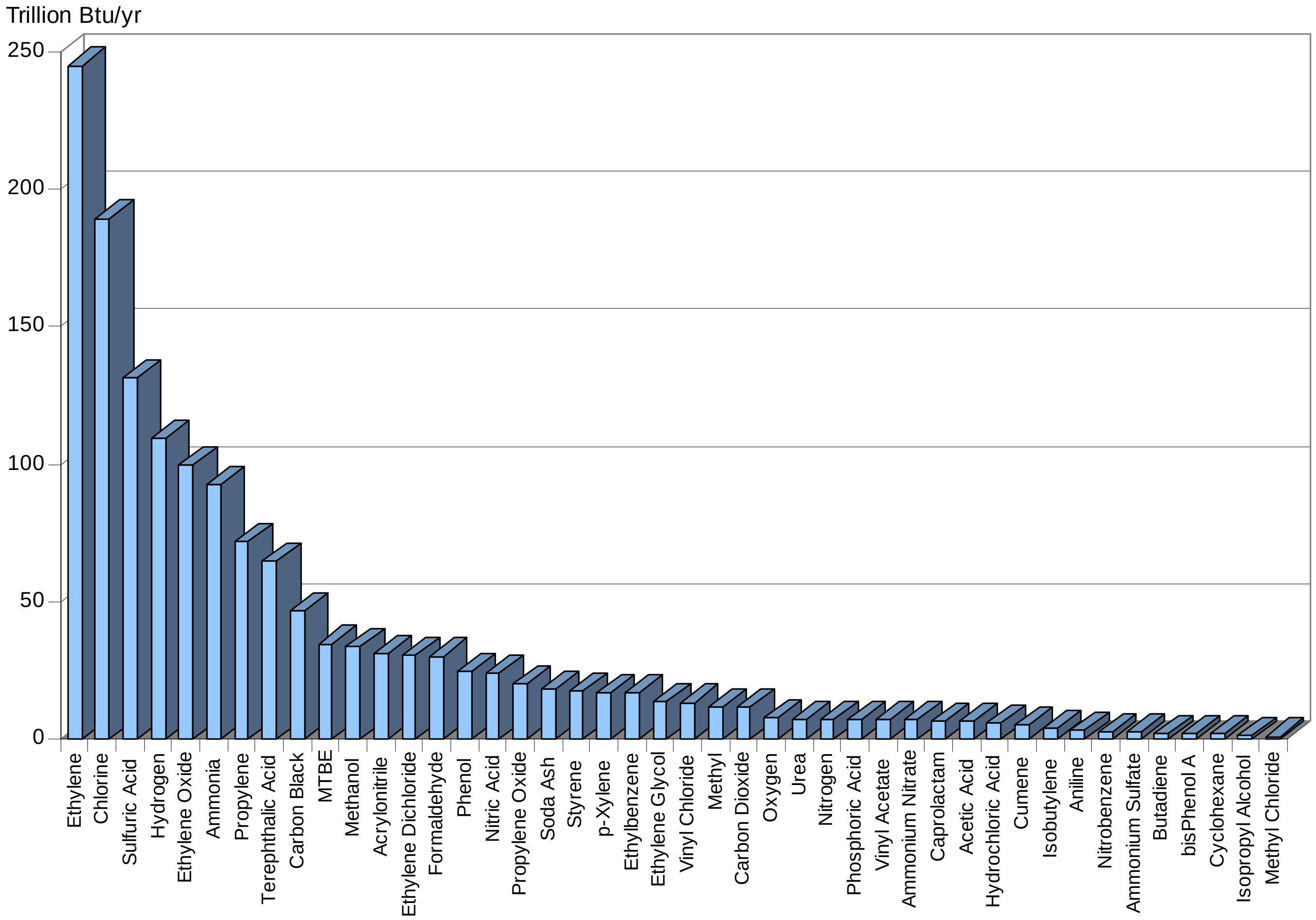
Energy - Fundamental quantity that every physical system possesses; it allows us to predict how much work the system could be made to do, or how much heat it can produce or absorb

Exergy – Work available or **Recoverable Energy** (High-quality energy that can be extracted from a flowing stream at high temperatures)

Exergy = Quality*Energy

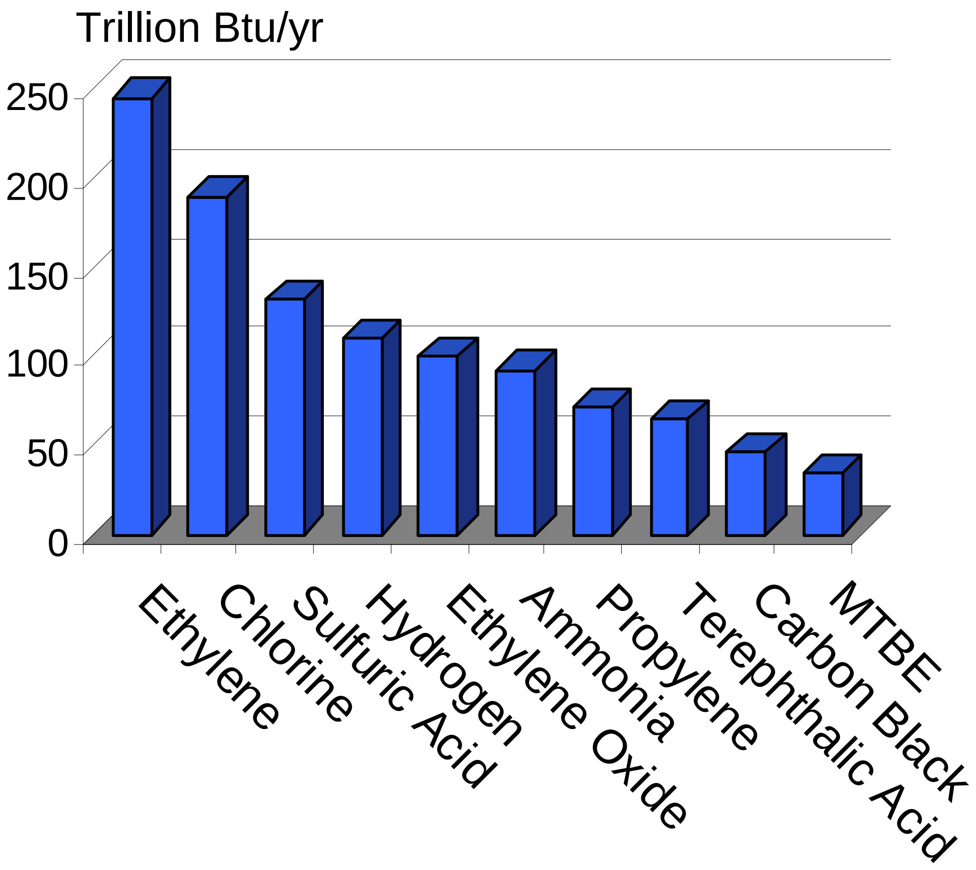
Non-recoverable Energy – Low quality energy that can be extracted from a flowing stream at low temperatures

Observation #1: --- Only a few chemical processes consume most of the energy!



Total Exergy Loss (Recoverable High Quality Energy)

Top Ten (~73% of Recoverable energy from all chemicals in study)



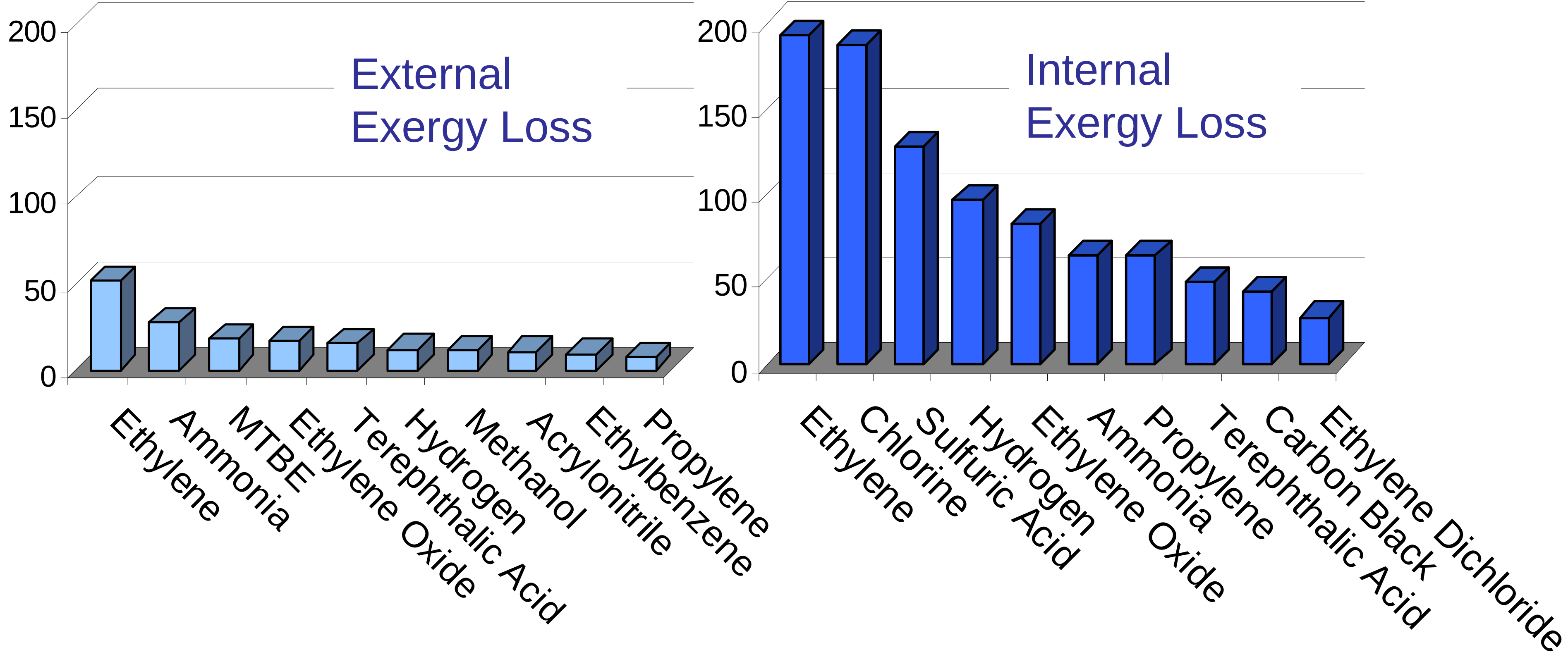
Observations #2:External vs. Internal Exergy Loss
(Best Practices, Equipment & Technology vs. R&D)

Top 10 = ~70% of external exergy loss from all chemicals in study

Top 10 = ~77% of internal exergy loss from all chemicals in study

Trillion Btu/yr

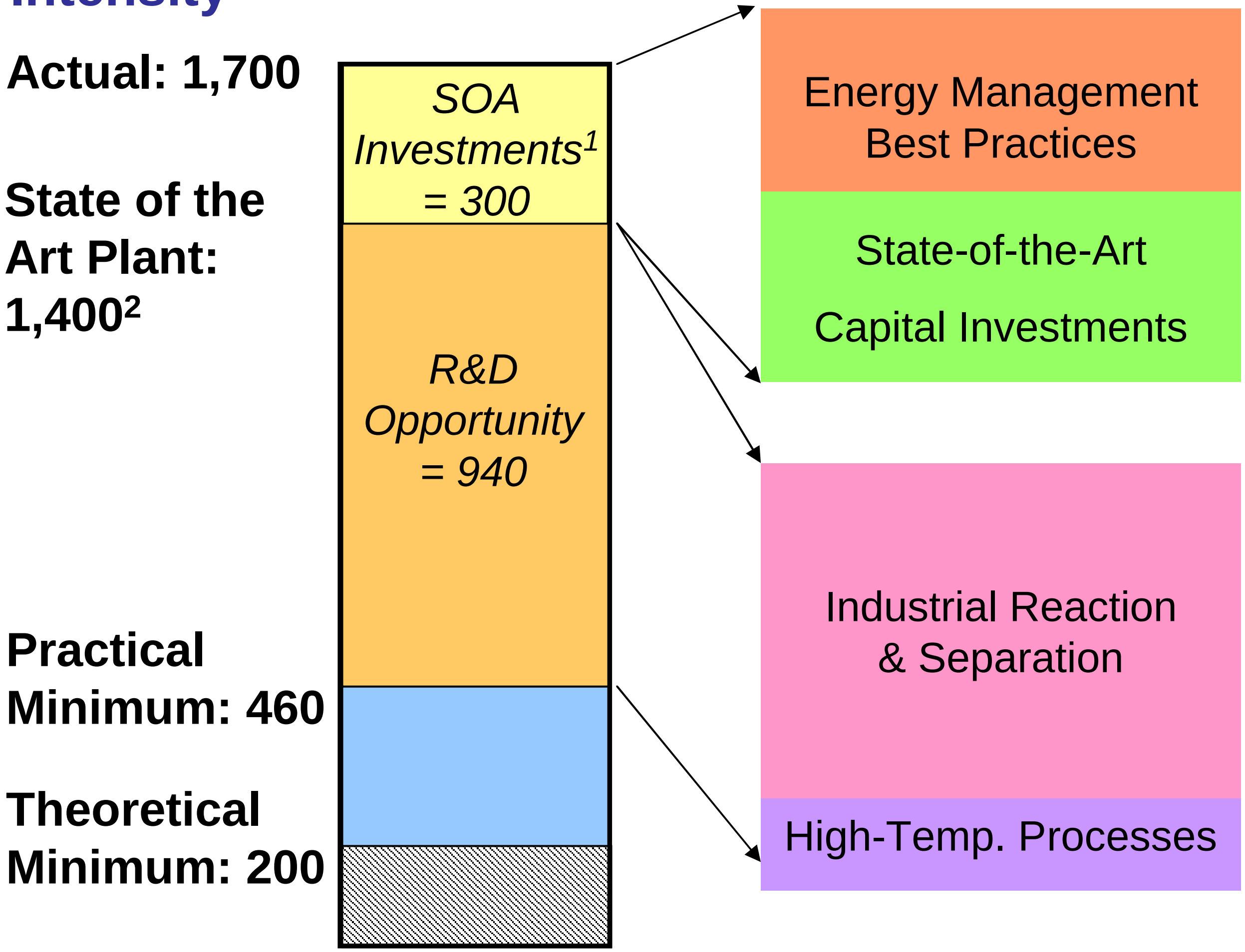
Focus Area #1: Alternative processes



Opportunities Identified via Bandwidth Study

2004 Energy Intensity

All values in trillion Btu/yr of chemical products*



Actual: 1,700

State of the Art Plant: 1,400[2]

Practical Minimum: 460

Theoretical Minimum: 200

SOA Investments[1] = 300

R&D Opportunity = 940

Energy Management Best Practices

State-of-the-Art Capital Investments

Industrial Reaction & Separation

High-Temp. Processes

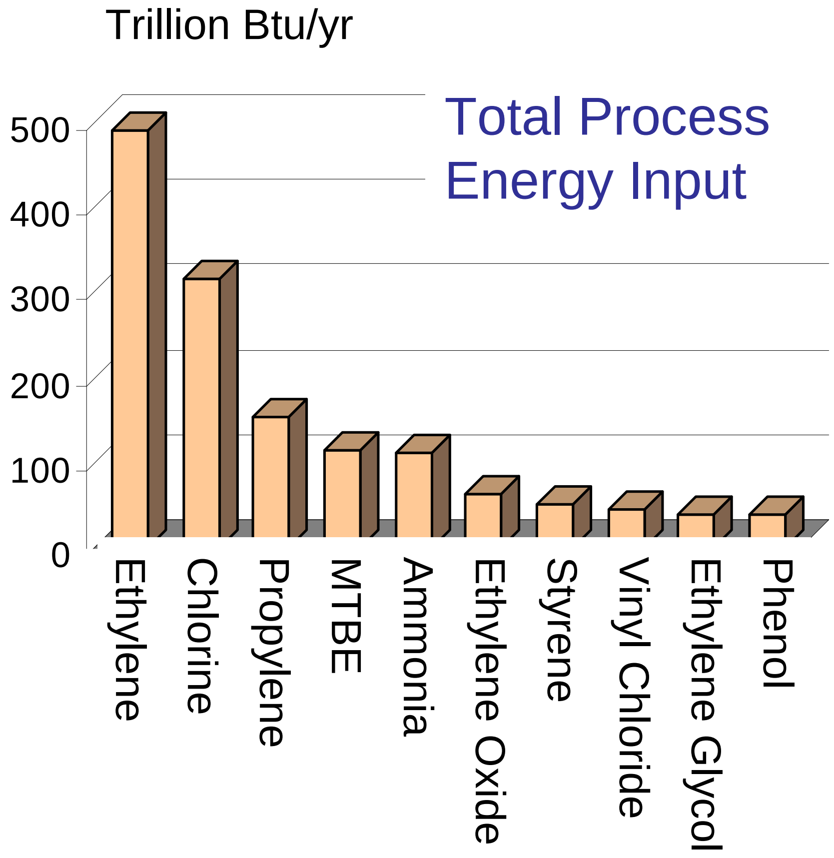
* Chemical products include 53 chemical studied in the Chemicals Bandwidth Analysis (e.g. ethylene, ammonia, etc)

[1] State of the Art (SOA) Investments include SOA Capital Investments and institution of Energy Management Best Practices

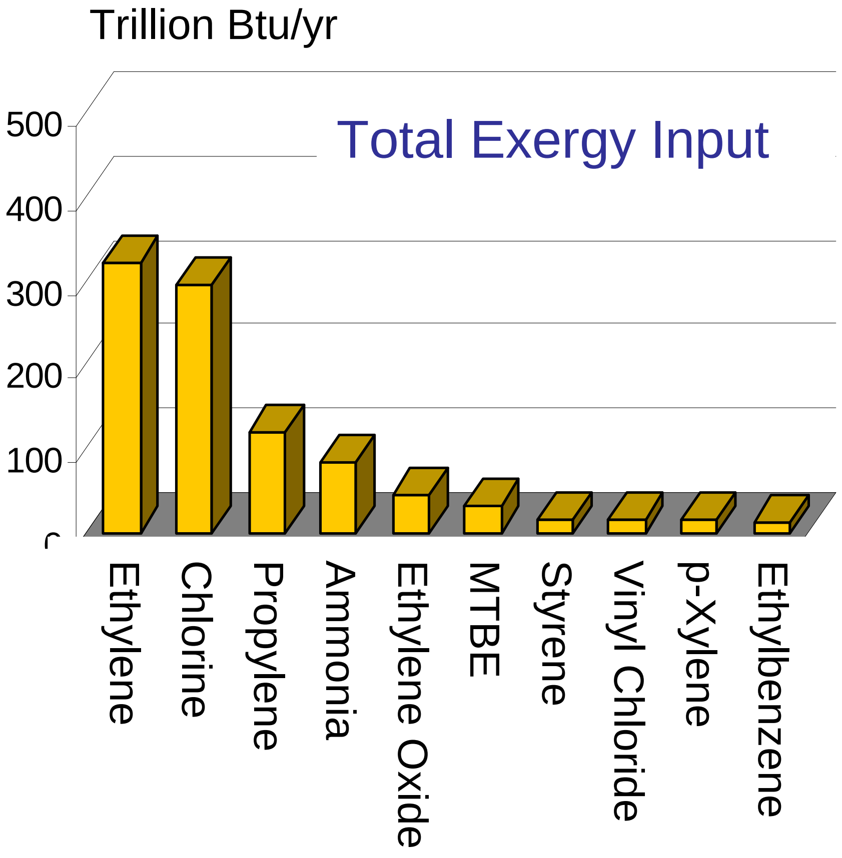
[2] Estimated

Ranking by Total Process Energy Input vs. Total Exergy Input

Top 10 = ~78% of energy input
from all chemicals in study



Top 10 = ~87% of exergy input
from all chemicals in study



Observations #3

Certain types of equipment accounted for most of the energy losses:

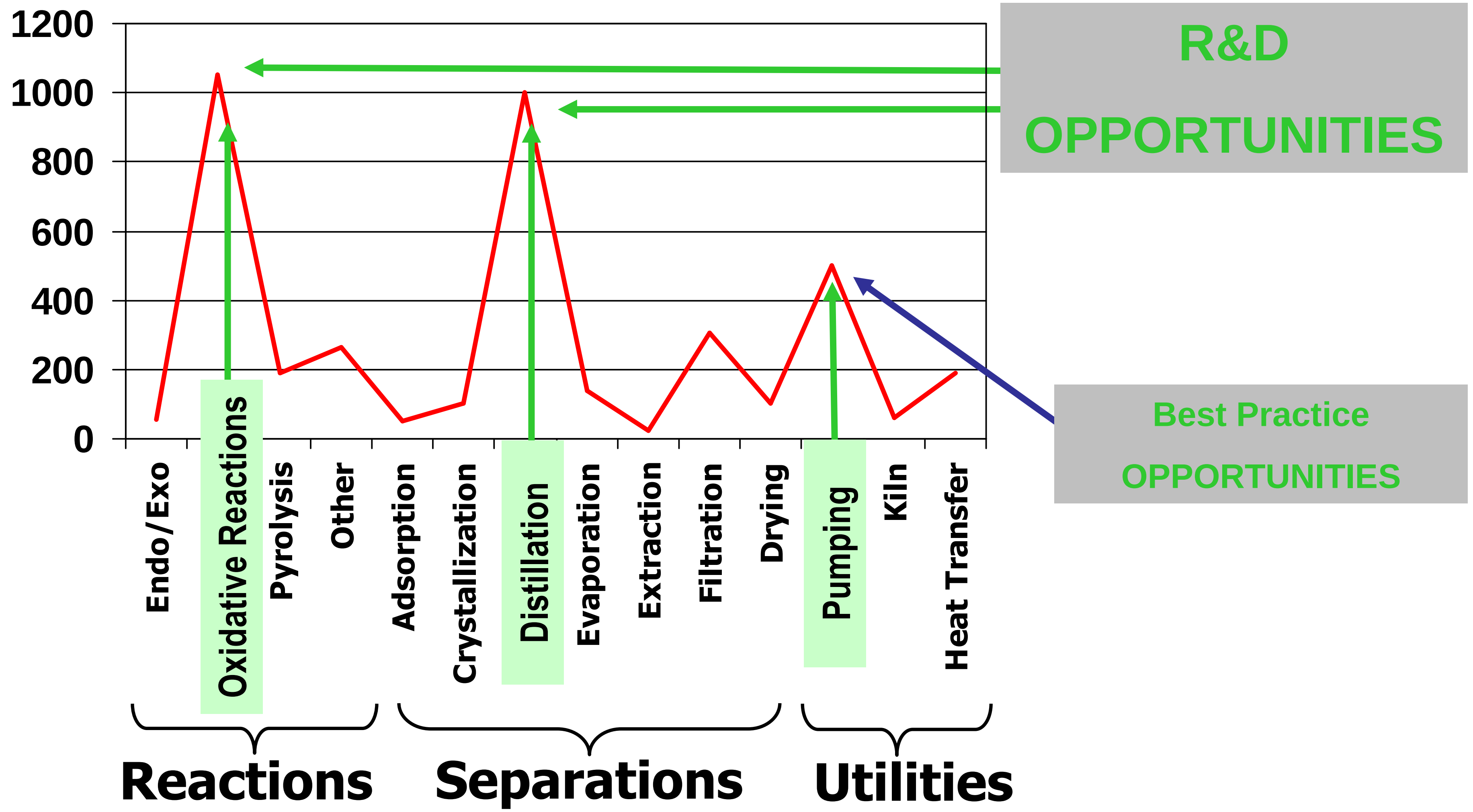
1. Heat exchangers, particularly in distillation columns, heat recovery, and cooling
2. Distillation Columns:
   - Reboilers
   - Condensers
3. Reactors: Some irreversibilties
   - Low selectivity
   - Poor heat integration
   - High-temperature reactions

Potential Solutions

Improved or novel separations technology (e.g., membrane, pressure swing adsorption, hybrid)

New design reactors with higher conversion efficiencies

Observations #4



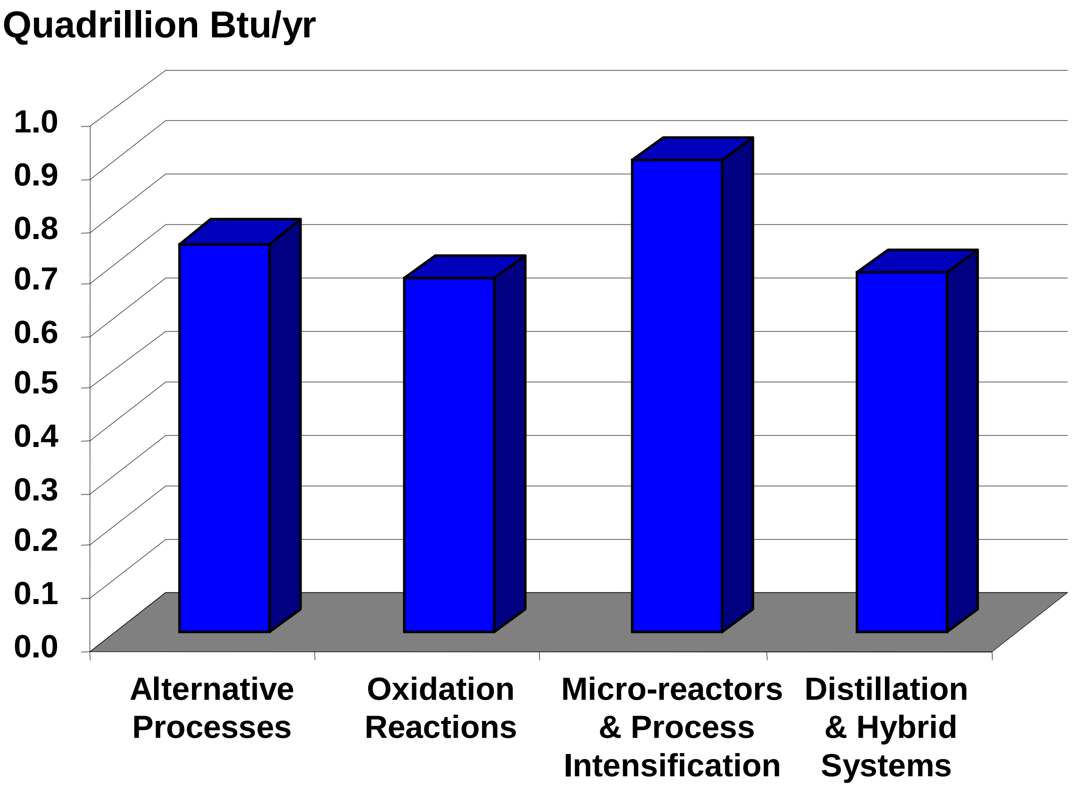
R&D

OPPORTUNITIES

Best Practice

OPPORTUNITIES

Total Internal Exergy Losses – Resulting Chemicals R&D Focus Areas



Contacts:

Dr. Dickson E. Ozokwelu
Phone: 202 586 8501
Fax: 202 586 9234

E-mail address: dickson.ozokwelu@ee.doe.gov
Website:http://www.eere.doe.gov/industry/chemicals/contacts.html

Chemicals Website: http://www.eere.doe.gov/industry/chemicals/portfolio.html

Thank You