

Two - Step Conversion of Ethanol to Butadiene

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Overview of Presentation

- **Project Background**
- **Process Breakdown**
- **Materials and Economics**
- **Closing Remarks**

Project Background

Two-Step Conversion of Ethanol to Butadiene

Butadiene Background

- **Technology used since 1940's**
- **Steam cracking from unsaturated hydrocarbon mixture**
- **One-Step vs. Two-Step Reactions**

One-Step Mechanism



1,3 Butadiene

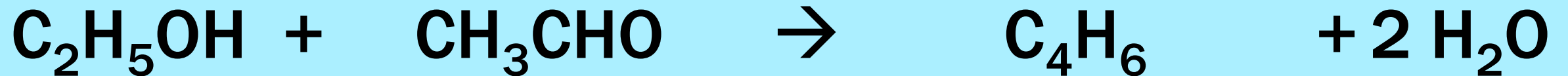
Two-Step Mechanism

1.) Ethanol \rightarrow Acetaldehyde + Hydrogen



Acetaldehyde

2.) Ethanol + Acetaldehyde \rightarrow 1,3 Butadiene + 2 Water



1,3 Butadiene

Two-Step Conversion of Ethanol to Butadiene

Proposal

- **The need:**
 - Oil prices can fluctuate drastically
 - Many uses
- **Butadiene can be created economically from ethanol as an alternative to crude oil**
 - Agricultural areas
 - Geologically unfavorable locations

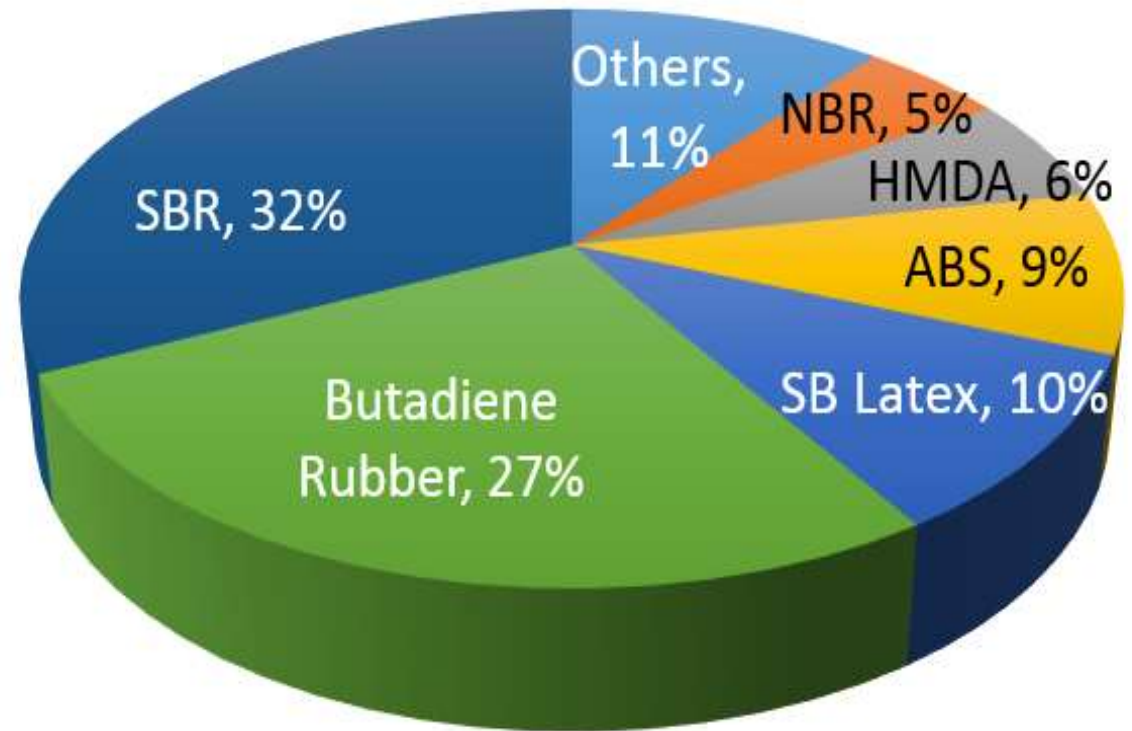
Business Opportunity

- **Growing demand**
- **Correlation with crude C4's**
- **Price Variance**
- **Price Reduction as addition to existing plant**
 - **Golden, Colorado**
 - **64.7 million gallons per year (gal/yr)**
 - **8410 operating hours per year (hr/yr)**

Butadiene Uses

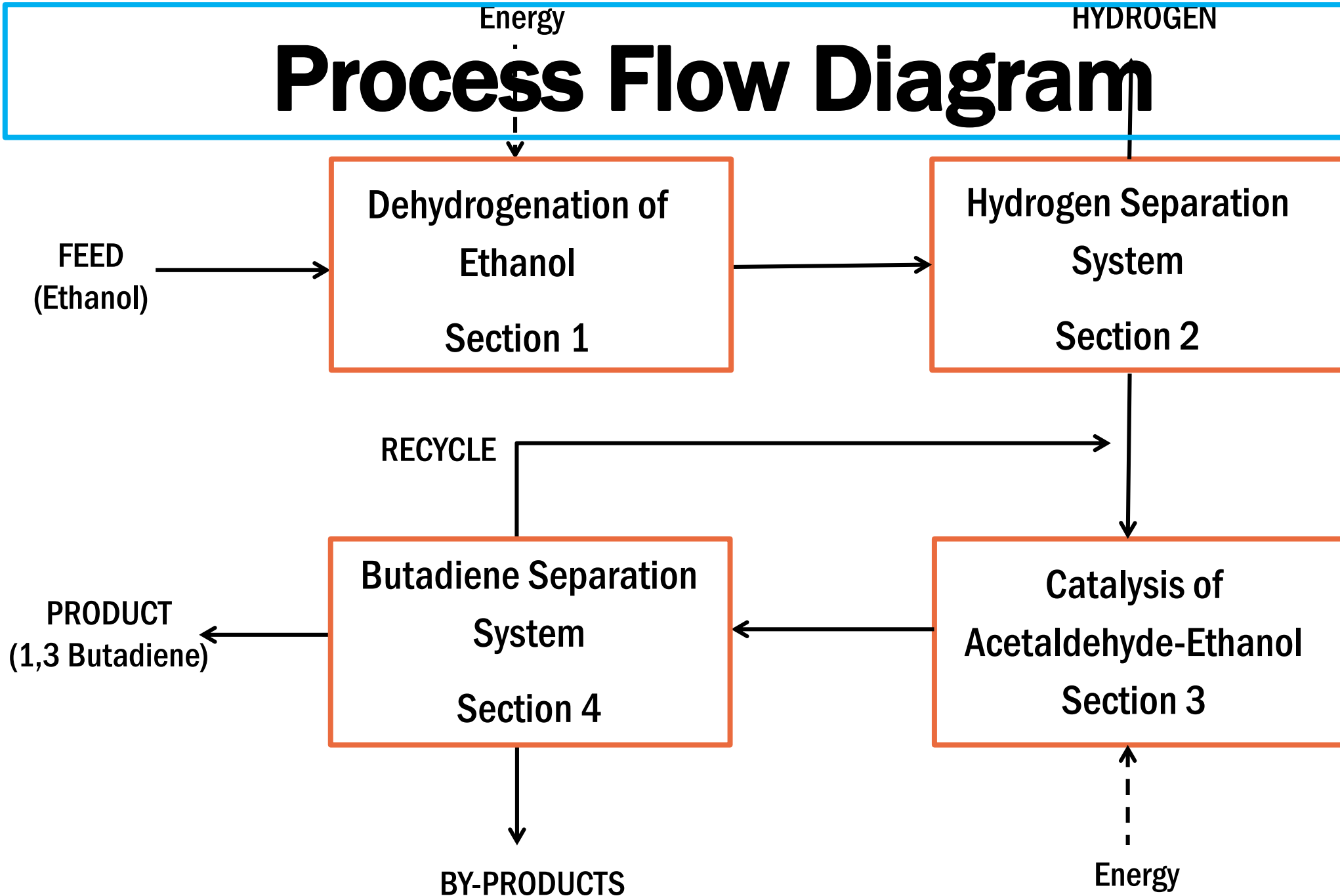
- Break-Down
 - Major Uses:
 - Rubber (Automobile tires)
 - Butadiene and SBR

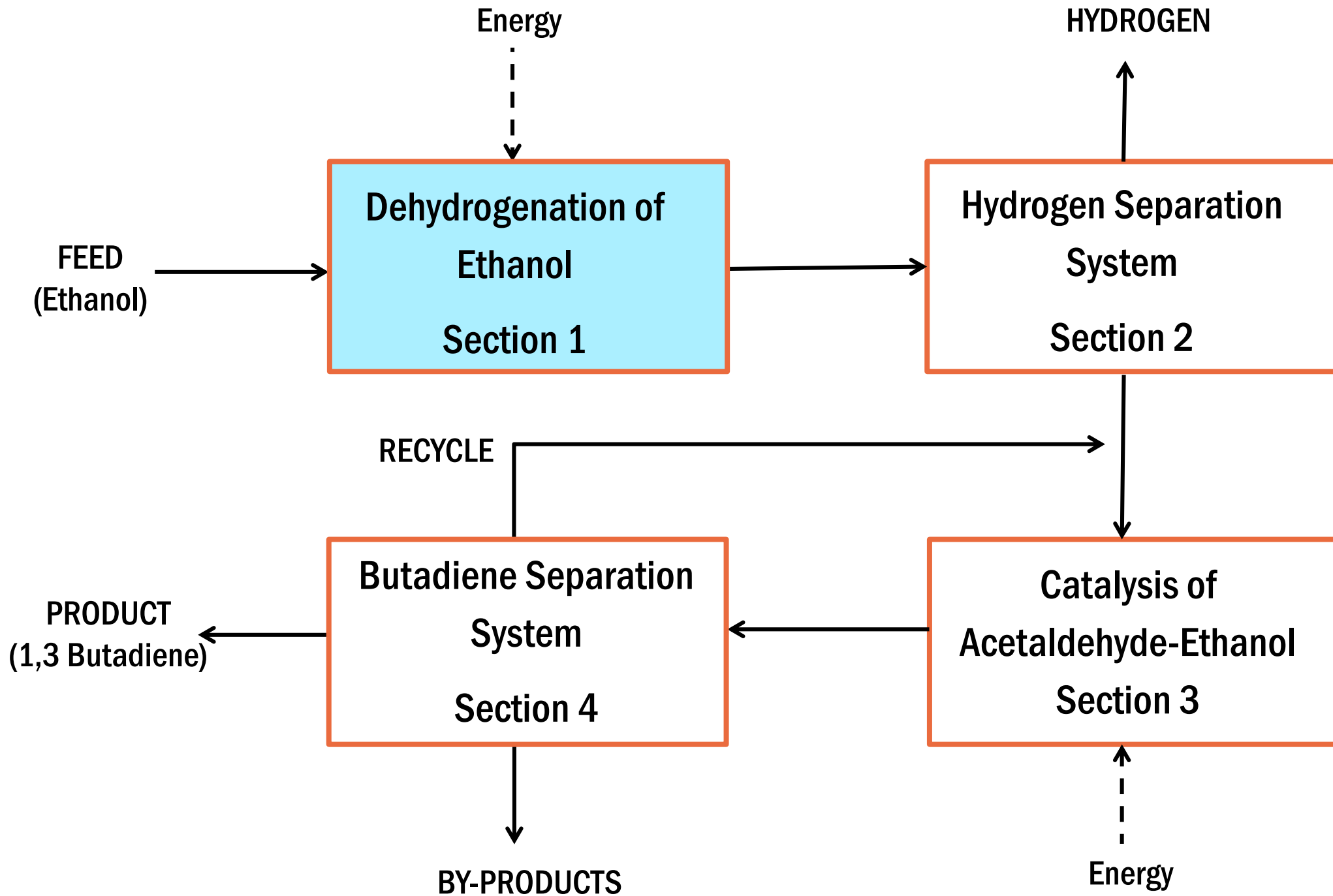
Global Butadiene Consumption Volumes by Application, 2011



Project Breakdown By Section

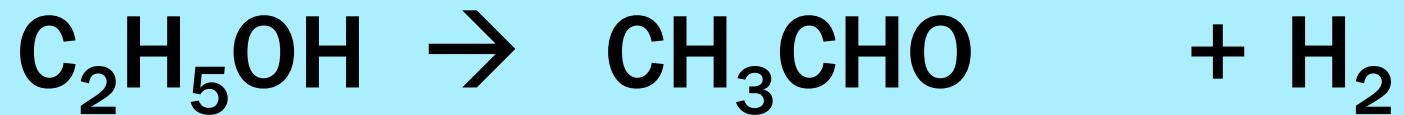
Process Flow Diagram





Section 1: Reactions

Ethanol \rightarrow Acetaldehyde + Hydrogen



2 Ethanol + Water \rightarrow Ethyl Acetate + 2 Hydrogen



Section 1: Reactor 1

Catalyst

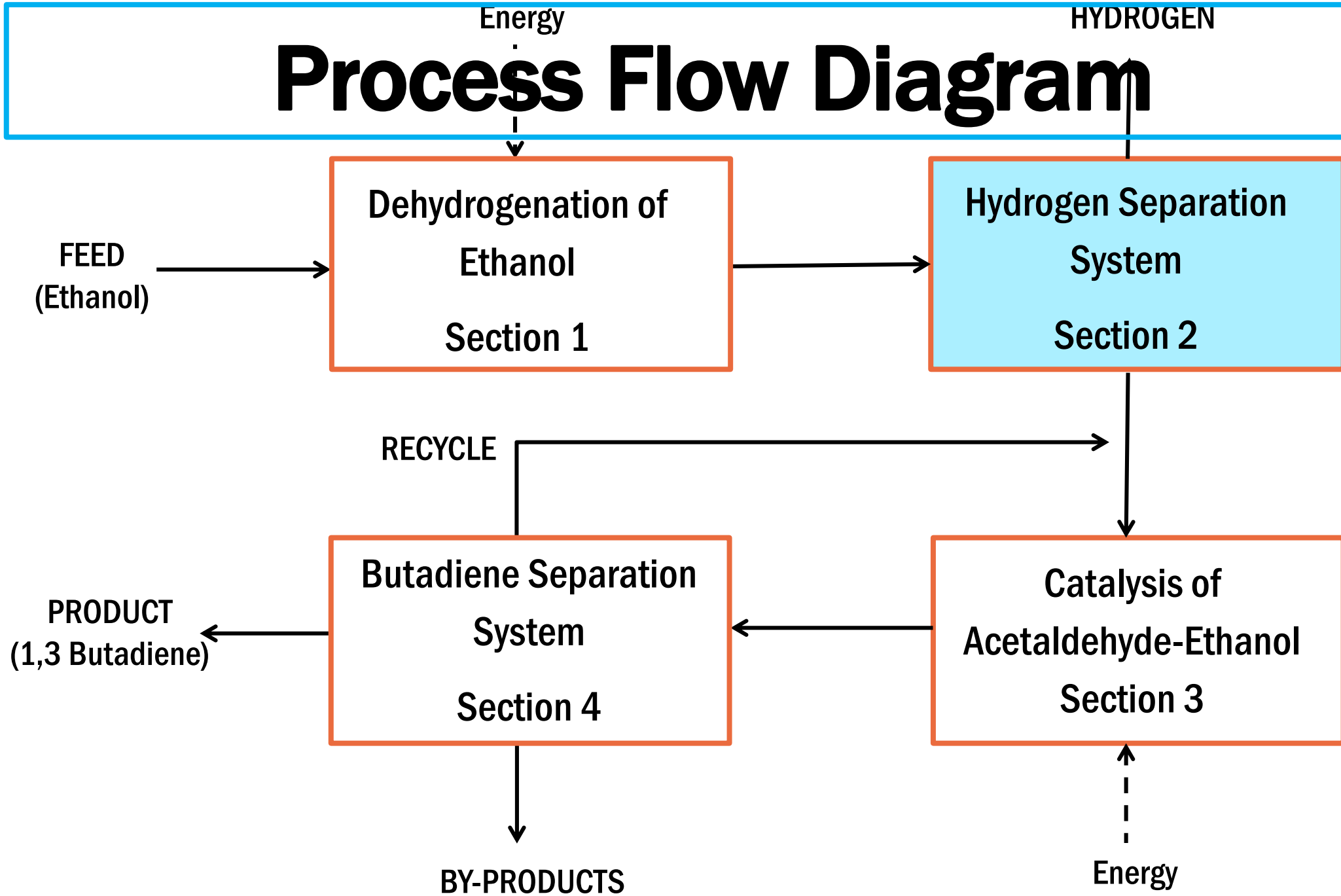
- **Catalyst: BASF K-310**
 - **CuO/ZnO/Al₂O₃**
- **Conversion of Ethanol: 52.7%**
- **Selectivity:**
 - **Acetaldehyde: 87.5%**
 - **Ethyl Acetate: 12.5%**

Specifications

- **Type: Packed Bed**
- **Temperature: 392°F**
- **Pressure: 14.7 psia**

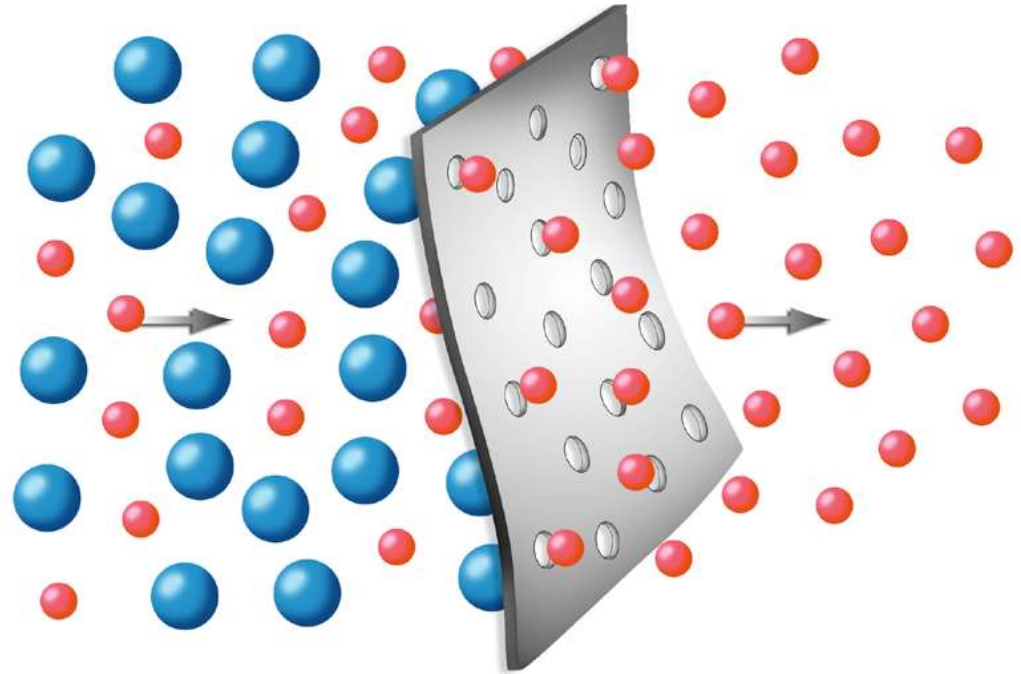
*Reference: E. Santacesaria, et. al.
ScienceDirect article.*

Process Flow Diagram

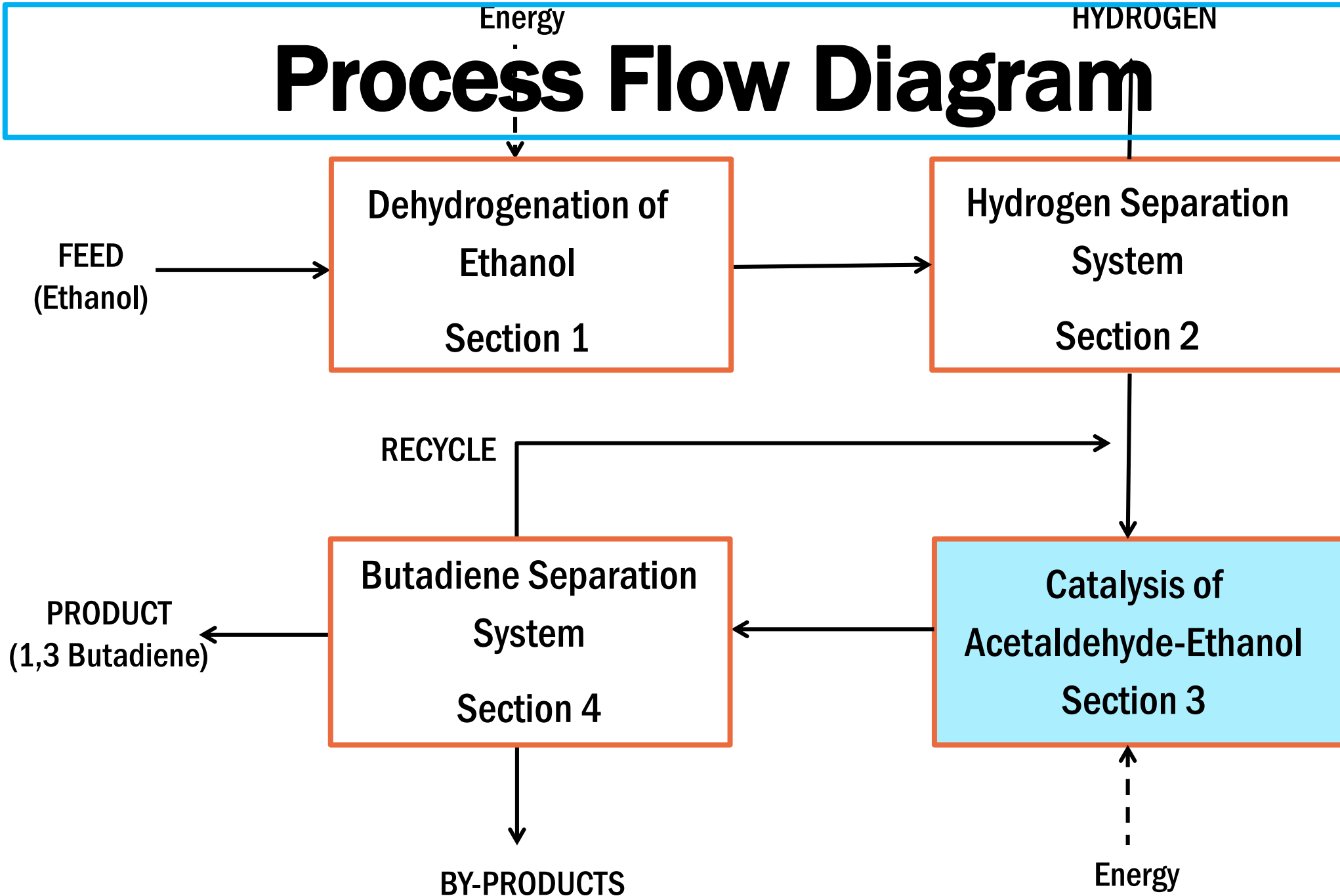


Section 2: Hydrogen Separation

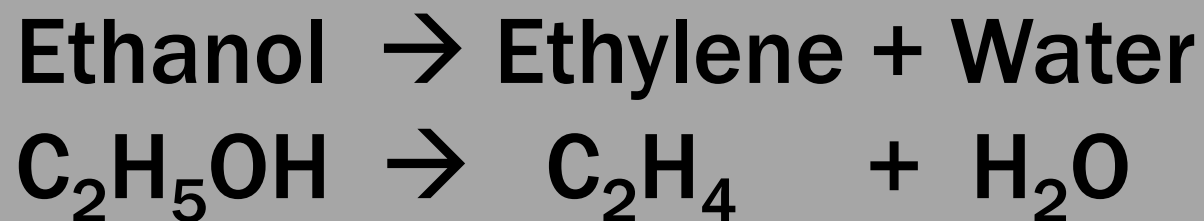
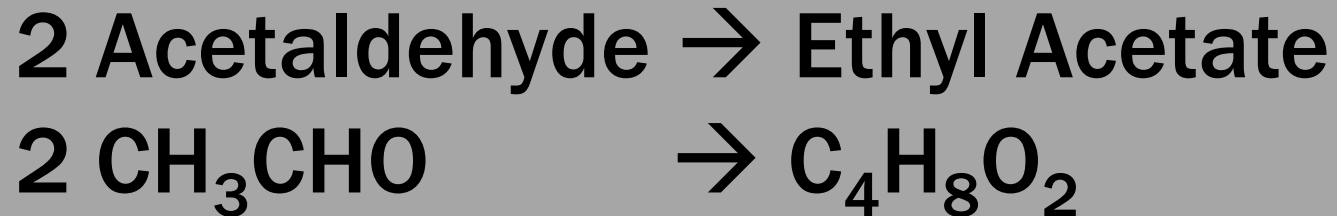
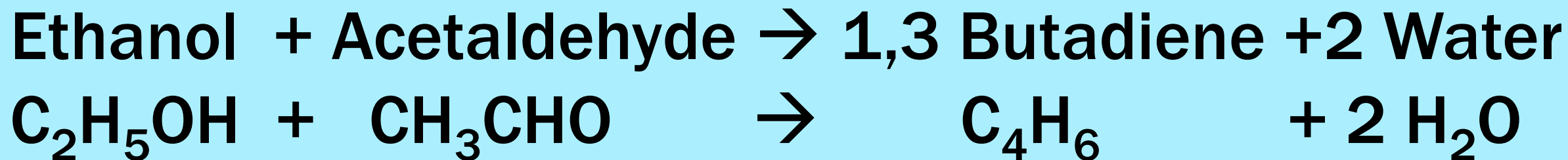
- Flash all H₂
- Purge vs. Purification
- Purification units
 - Membrane vs. PSA



Process Flow Diagram



Section 3: Reactions



Section 3: Reactor 2

Catalyst

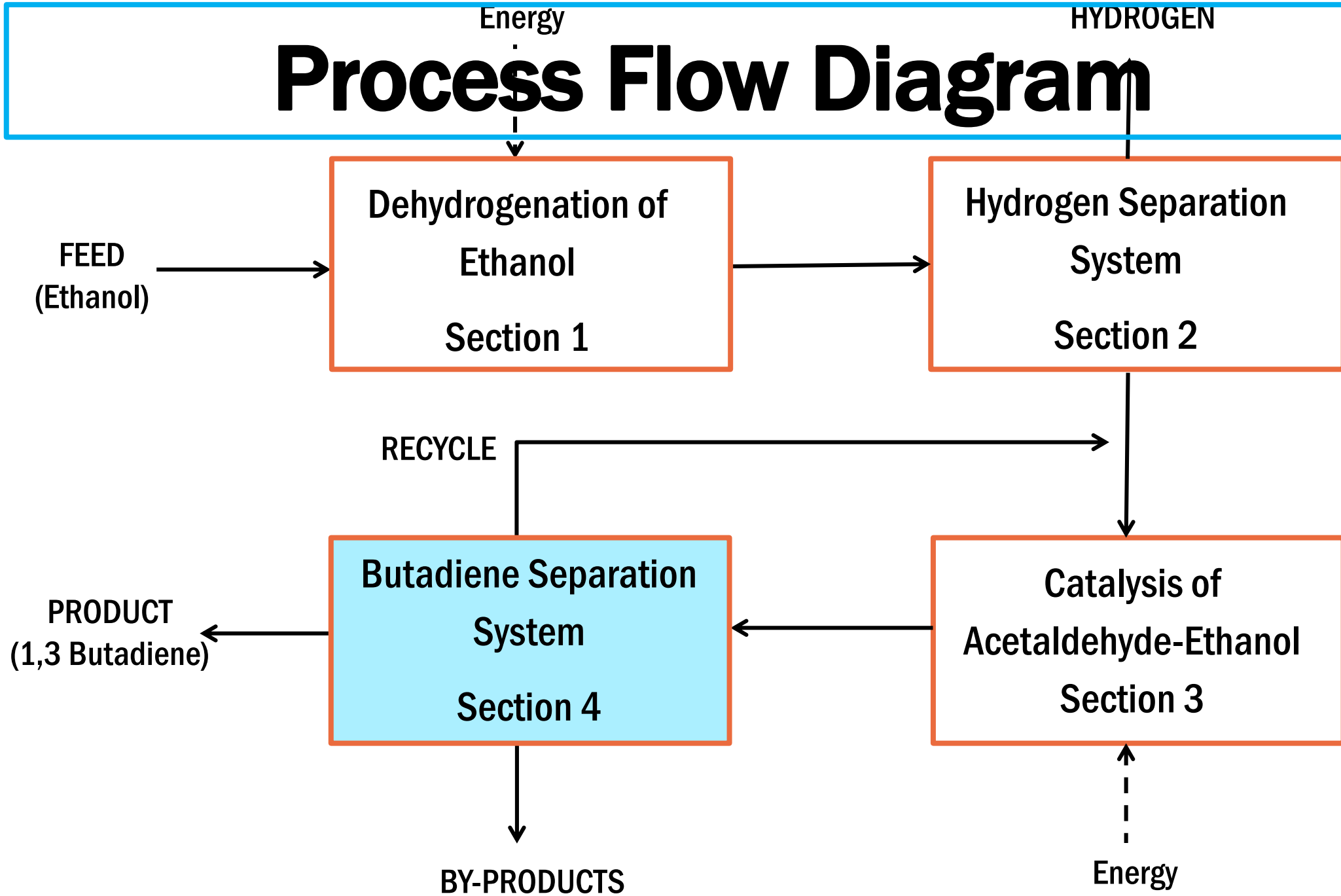
- Catalyst:
 - MgO/SiO₂
- Conversion of Ethanol and Acetaldehyde: 48%
- Selectivity:
 - Butadiene: 68%
 - Ethylene: 26%
 - Ethyl Acetate: 9%

Specifications

- Type: Packed Bed
- Temperature: 662°F
- Pressure: 14.7 psia

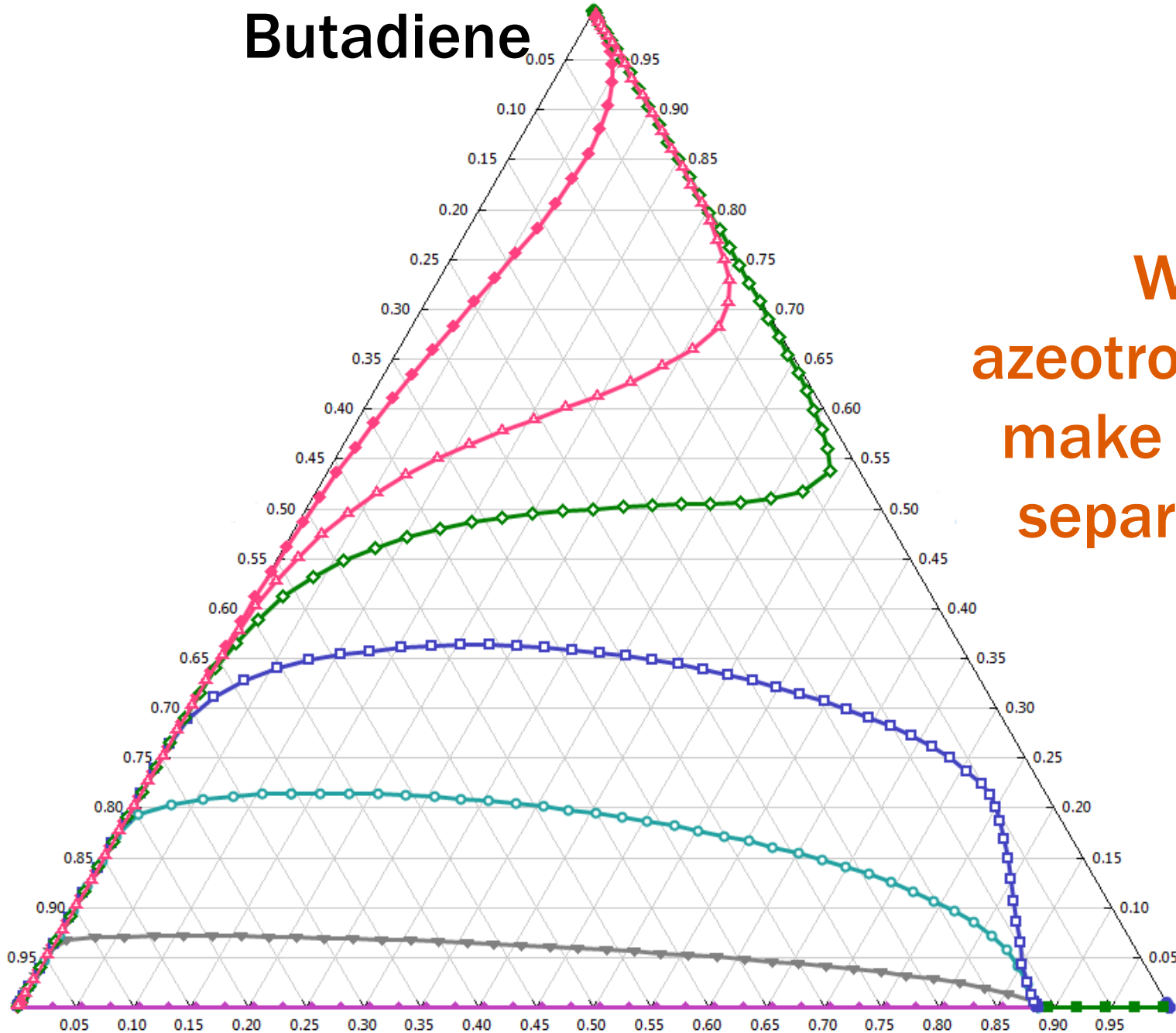
Reference: Kvisle, et. al. ScienceDirect

Process Flow Diagram





Butadiene

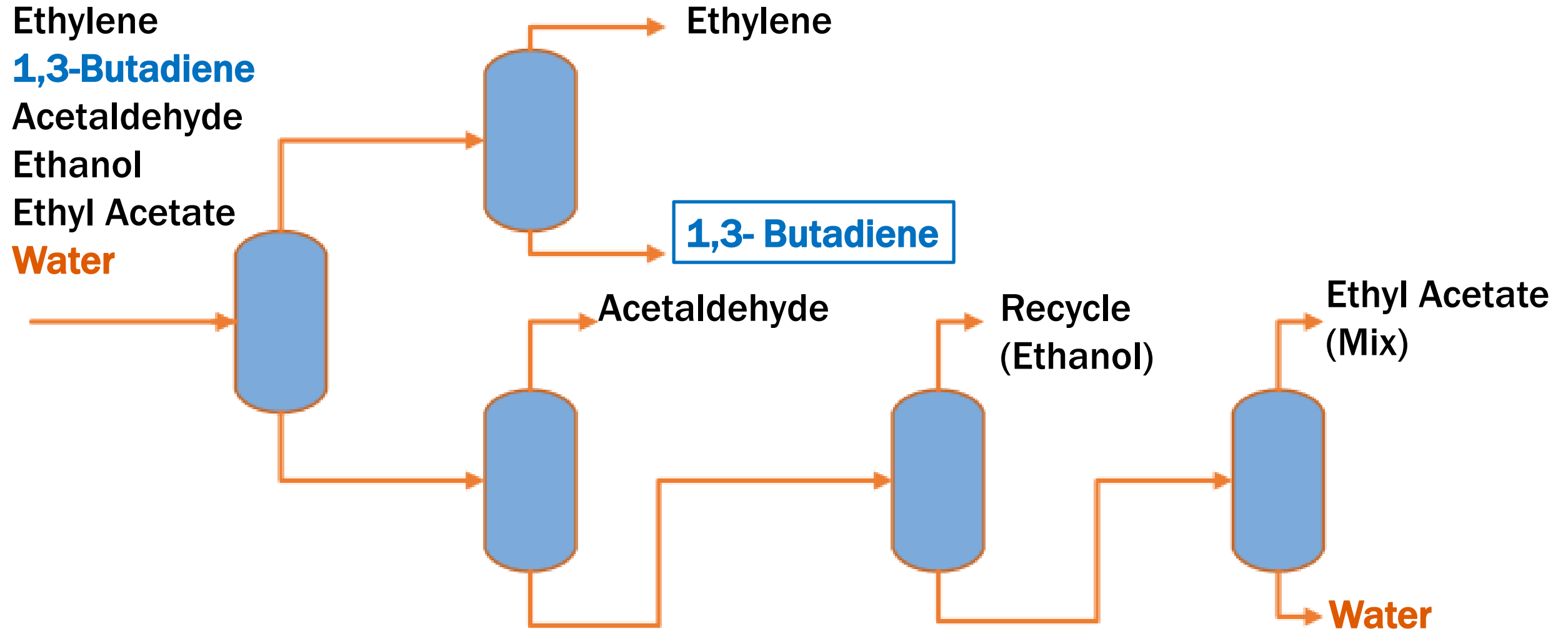


Wide variety of azeotropes proves to make modeling our separation process difficult

Water

Acetaldehyde

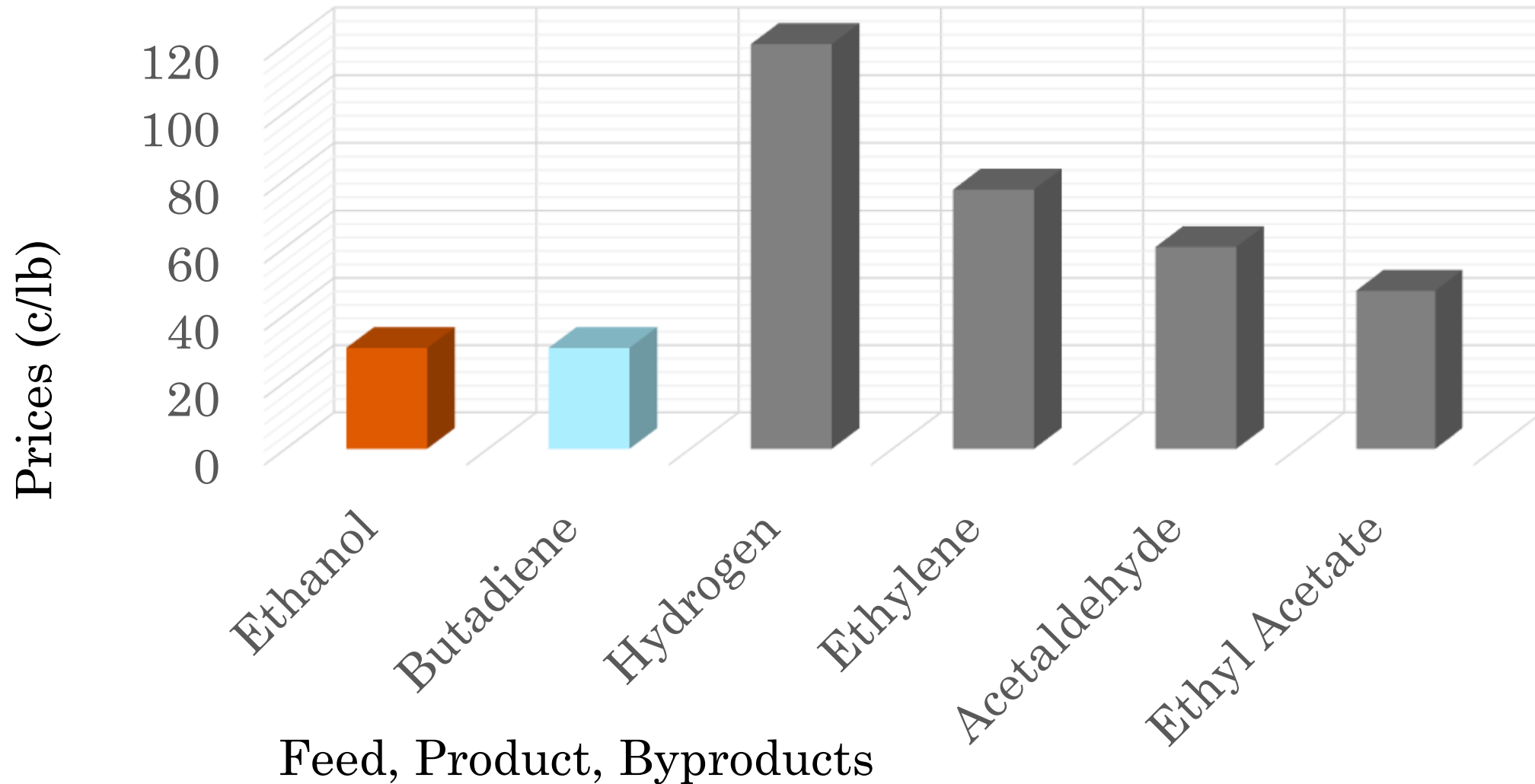
Section 4: Separation System



Materials and Economics

Two-Step Conversion of Ethanol to Butadiene



Markets For (By)Products



Feed, Product, Byproducts

Two-Step Conversion of Ethanol to Butadiene

Economics

- **Fixed Capital Investment (FCI): \$ 141 MM**
- **Operating Costs (OC): \$ 65.78 MM/yr**
- **Minimum Acceptable Rate of Return (MARR): 10%**
 - **Price of Butadiene: 65.77 c/lb**
- **Sensitivities**
 - **+10% FCI**  **67.77 c/lb**
 - **+10% OC**  **70.20 c/lb**

Economics

	Aug 2013		March 2014
Butadiene, c/lb	42.50	65.77	73.40
Revenue, MM\$/yr	60.71	93.95	104.85
NPV10, MM\$	-147.92	0.02	48.53
IRR, %	N/A	10.00	14.20
Pay Back Period, yrs	N/A	15	9.10

- **Discount Rate = 10%**

Closing Remarks

Final Conclusions

- **We used a two-step mechanism**
- **Multiple azeotropes make separation difficult**
- **Our process is not favorable in the current market**

Acknowledgements

A special “thank-you” to:

Dr. John Myers

and

Dr. Joseph Holles

References

• Mentioned specifically in the PowerPoint:

1. Acquaviva, Jim. "High-Performance, Durable, Palladium Alloy Membrane for Hydrogen Separation and Purification." 19 May 2009. Web. 7 Dec. 2014. <http://www.hydrogen.energy.gov/pdfs/review09/pd_07_acquaviva.pdf>.
2. Kvisle, S., A. Agüero, and R.P.A. Sneed. "Transformation of Ethanol into 1,3-butadiene over Magnesium Oxide/silica Catalysts." *ScienceDirect*. 1 Jan. 1988. Web. 24 Oct. 2014. <<http://www.sciencedirect.com/science/article/pii/S0166983400809057#>>.
3. "Butadiene price rises by third." *Supply Management*. 19 Mar. 2014. Web. 01 Dec. 2014. <<http://www.icis.com/Articles/2012/01/16/9523382/US-Chemical-profile-Butadiene.html>>
4. Santacesaria, E., Carotenuto, G., Tesser, R. Di Serio, M., "Ethanol Dehydrogenation to Ethyl Acetate by Using Copper and Copper Chromite Catalysts." *ScienceDirect*. 1 Jan. 2012. Web. 22 Oct. 2014. <<http://www.sciencedirect.com/science/article/pii/S1385894711012824>>.

Questions?



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