The Use of Life Cycle Assessment as a Screening Tool for Environmental Performance:

Supercritical Carbon Dioxide Use in the Semiconductor Industry

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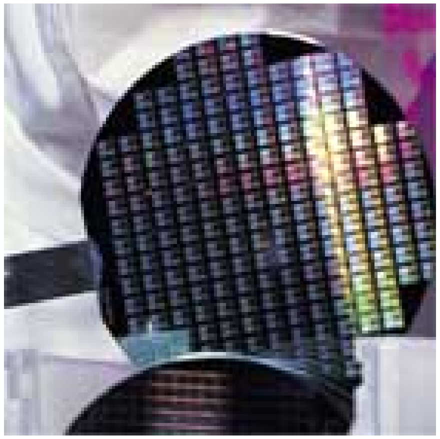


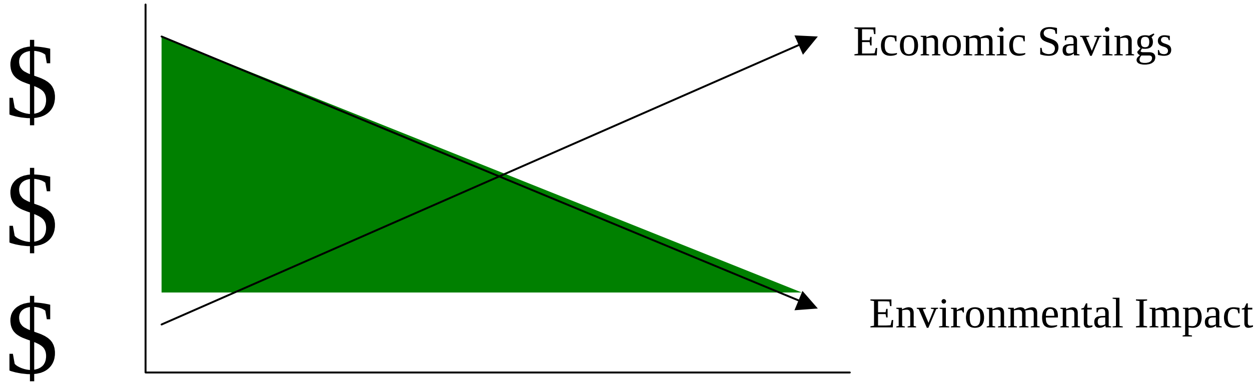
NSF/SRC Engineering Research Center for Environmentally Benign Semiconductor Manufacturing

Environmental/Economic Drivers for Process Innovation

Pollution treatment never makes money for the company running the processes

However, large savings can be made by avoiding the need for treatment in the first place

Considerations like these must take place at the design stage to be most effective



Get a reduction in costs while also improving the environmental performance of a process

Win/Win situations are possible

Attractiveness of supercritical fluids in process applications

Can avoid organic solvents that are traditionally used in separations/reactions

- less ozone depletion, toxicity, cost, separations, fossil fuel depletion

Can tune performance of sc fluids for enhanced properties

- better reaction selectivity → separations afterwards
- better or changeable solvent properties → less solvent need, better separations

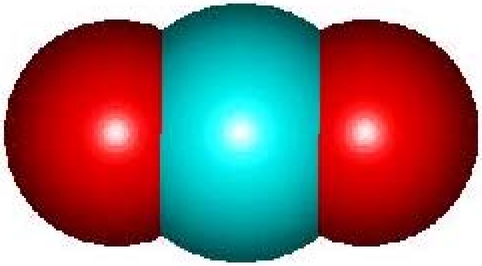
Can use small amounts of additives to achieve better performance

- sometimes 100% recyclable → less cost

So, which fluids may be useful for semiconductor processing?

$scCO_2$ as a good choice? And, use of additives…

CO_2 is attractive for many reasons:



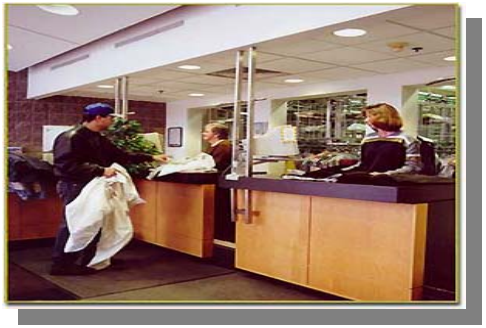
Its critical region is at fairly low pressures and temperatures compared to other materials → lower environmental and economic costs during its use

Using CO_2 may reduce overall CO_2 generation from other facilities depending on the source.

It has been used in many other industries so it is more familiar, may need additives.

Fragrance Extraction

Dry cleaning application



Remove bitterness from beer

Roadmap of ITRS

The International Technology Roadmap for Semiconductors (ITRS) is a plan for achieving better environmental, technical, and economic performance over the next several years and is continually updated.

ITRS says:

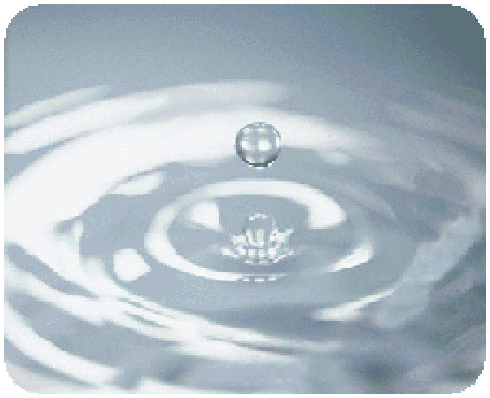
Develop processes that meet technology demands while reducing impacts

Develop effective management tools to deal with disposal

Design more energy and water efficient processing equipment

Reduce emissions from processing using GWP chemicals

Need integrated way to evaluate and quantify ESH impacts

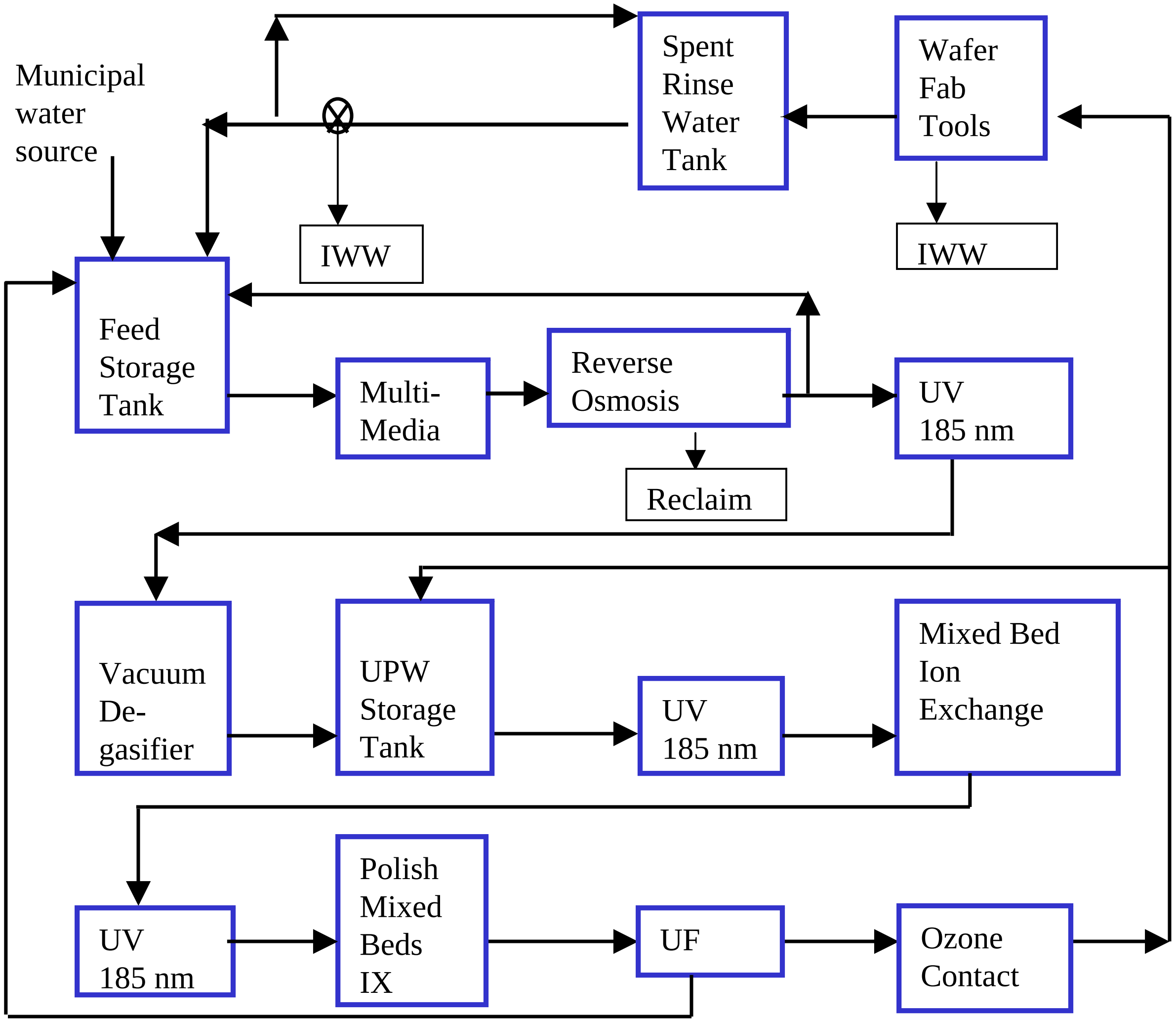


Specifically, reduce water usage by about 20% over the next three years

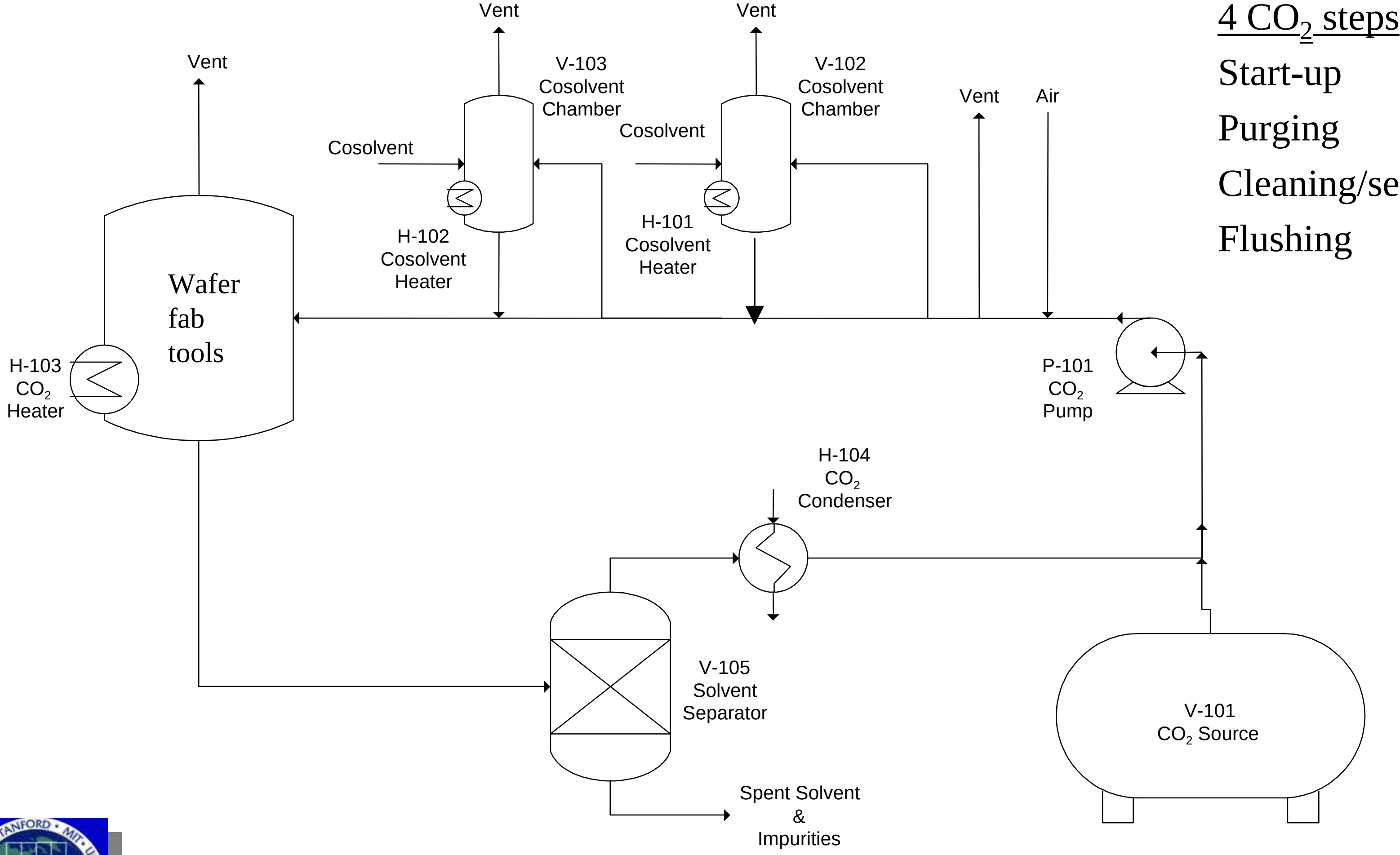
Reduce energy usage by about 40-50 % over the next three years

Photoresist removal and current process with water

>226,944 gallons per day for a small plant



Photoresist removal and supercritical CO_2 usage



4 CO_2 steps

Start-up

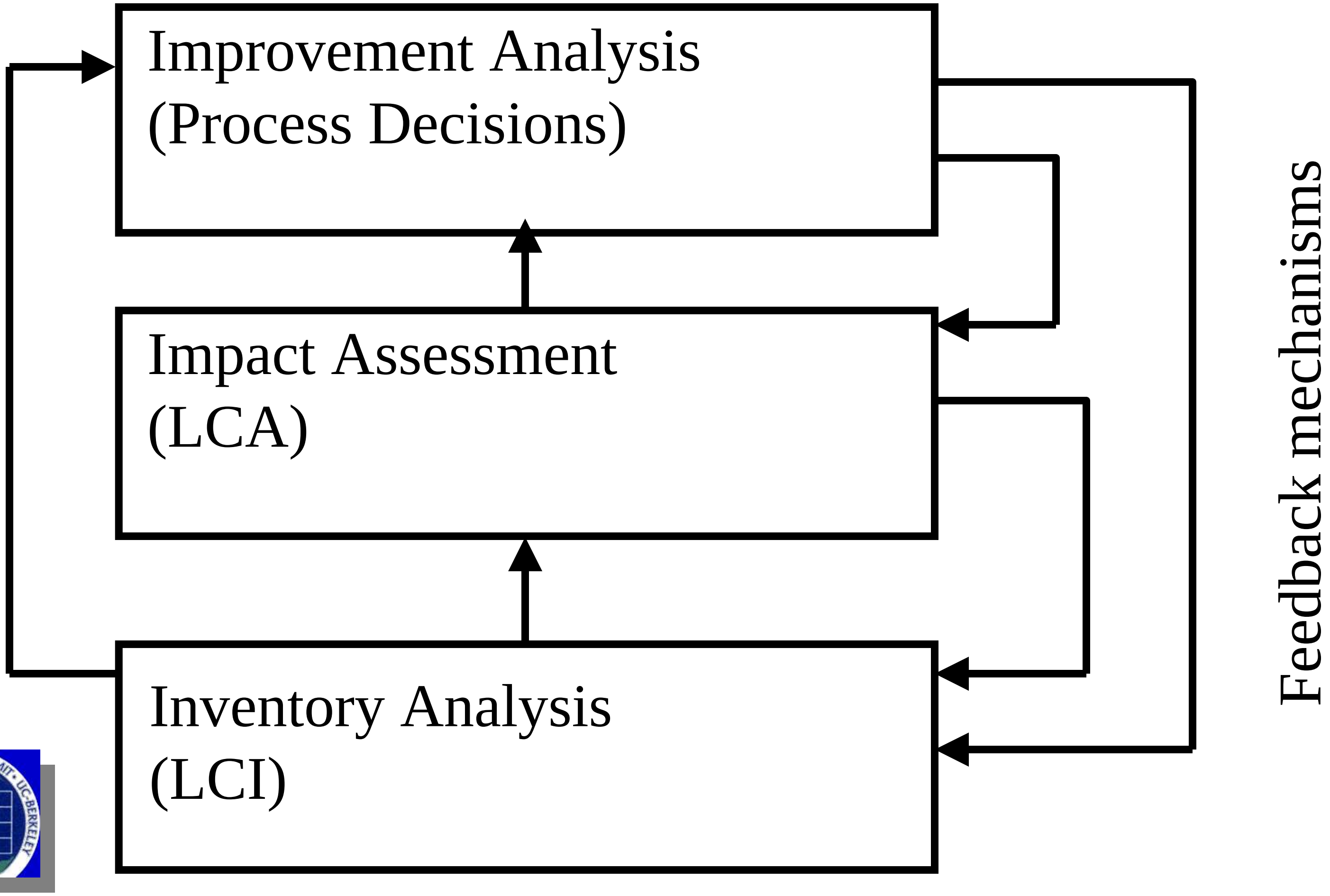
Purging

Cleaning/separating

Flushing

Environmental Assessment Tools

Stage of Information Development



Improvement Analysis
(Process Decisions)

Impact Assessment
(LCA)

Inventory Analysis
(LCI)

Feedback mechanisms

First Step to Generating an LCA

LCI comes before LCA in the information chain

Need to set boundaries of the investigation

Can impact results so clear boundaries are needed

This is a Gate-to-Gate study

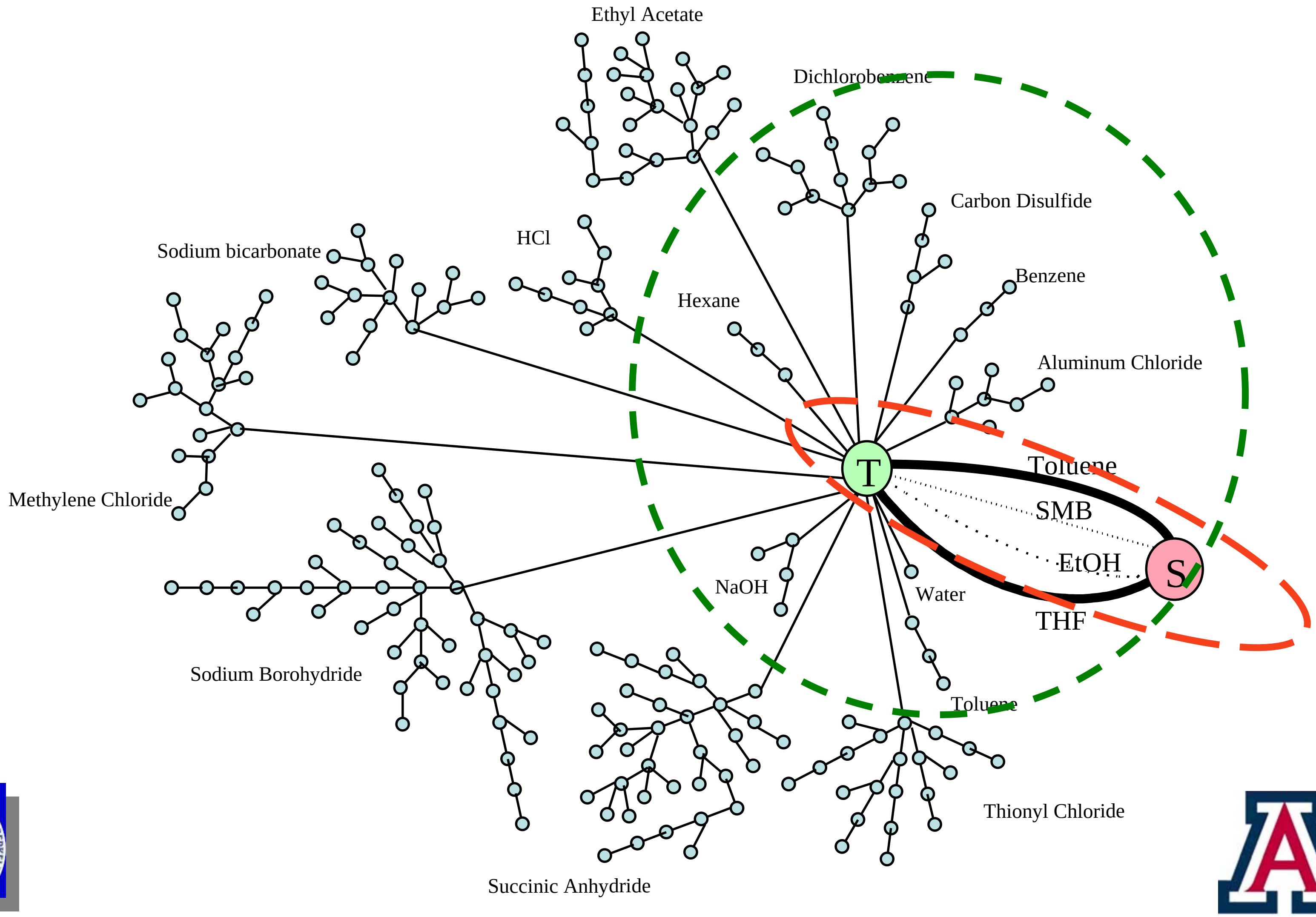
Does not quantify upstream information

Does not quantify downstream information

Disposal of ion exchange resins (UPW)

This LCI will quantify materials usage for consumables, but not equipment (more important for UPW) and will quantify energy needed for each wafer per cleaning cycle

Importance of Boundaries



LCI - Gate to Gate and Limitations

Limitations to LCI only approach

- No impacts yet - decisions may not be clear if there are conflicting environmental results
- No economics yet - can be addressed by COO but requires more information
- No upstream information - supplier concerns and deciding whether or not the gate-to-gate improvement is actually better overall
- No post-use information - customer concerns and deciding whether impacts may be generated outside the factory boundary

Benefit = speed and still getting useful data

LCI - Gate to Gate

Upstream sources and contributions to overall environmental impacts

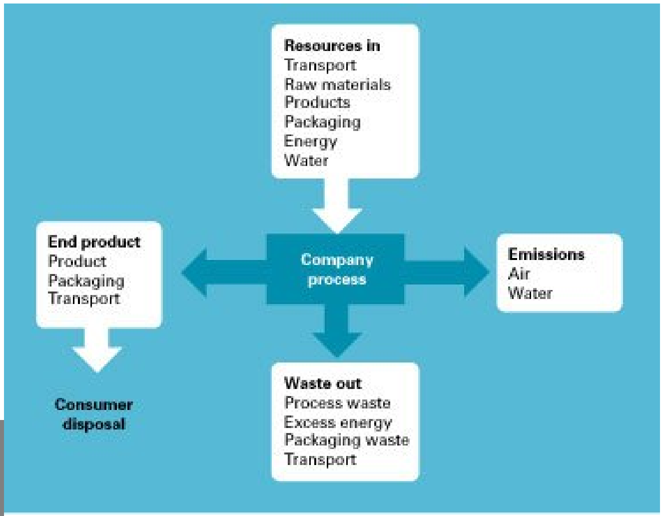
scCO$_2$/UPW use in plant, all internal uses quantified

Downstream disposal

Cradle

Gate to Gate

Grave



Can build and verify Gate to Gate LCI/LCA faster due to the large decrease in required information.

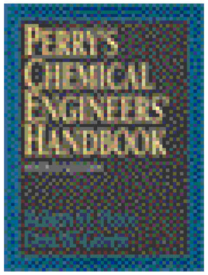
Future work will expand the boundaries…more later about those impacts

Basis for numbers reported in this work: Assumptions and sources of data

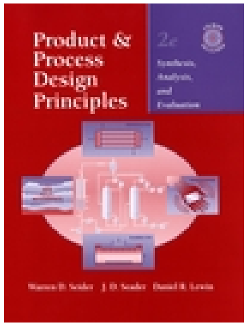
US Patents Used: 6,306,564; 6,509,141; 6,319,410; 6,509,141; 6,562,146; 6,558,475

(patents can be vague →uncertainties in info. Can be handled by methods introduced by McRae, MIT)

Physical properties from NIST Webbook, CRC Handbook of Chemistry and Physics, Perry's Handbook.

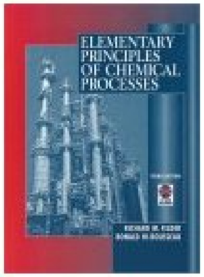


Design heuristics from Seider, *et al.* (1999).

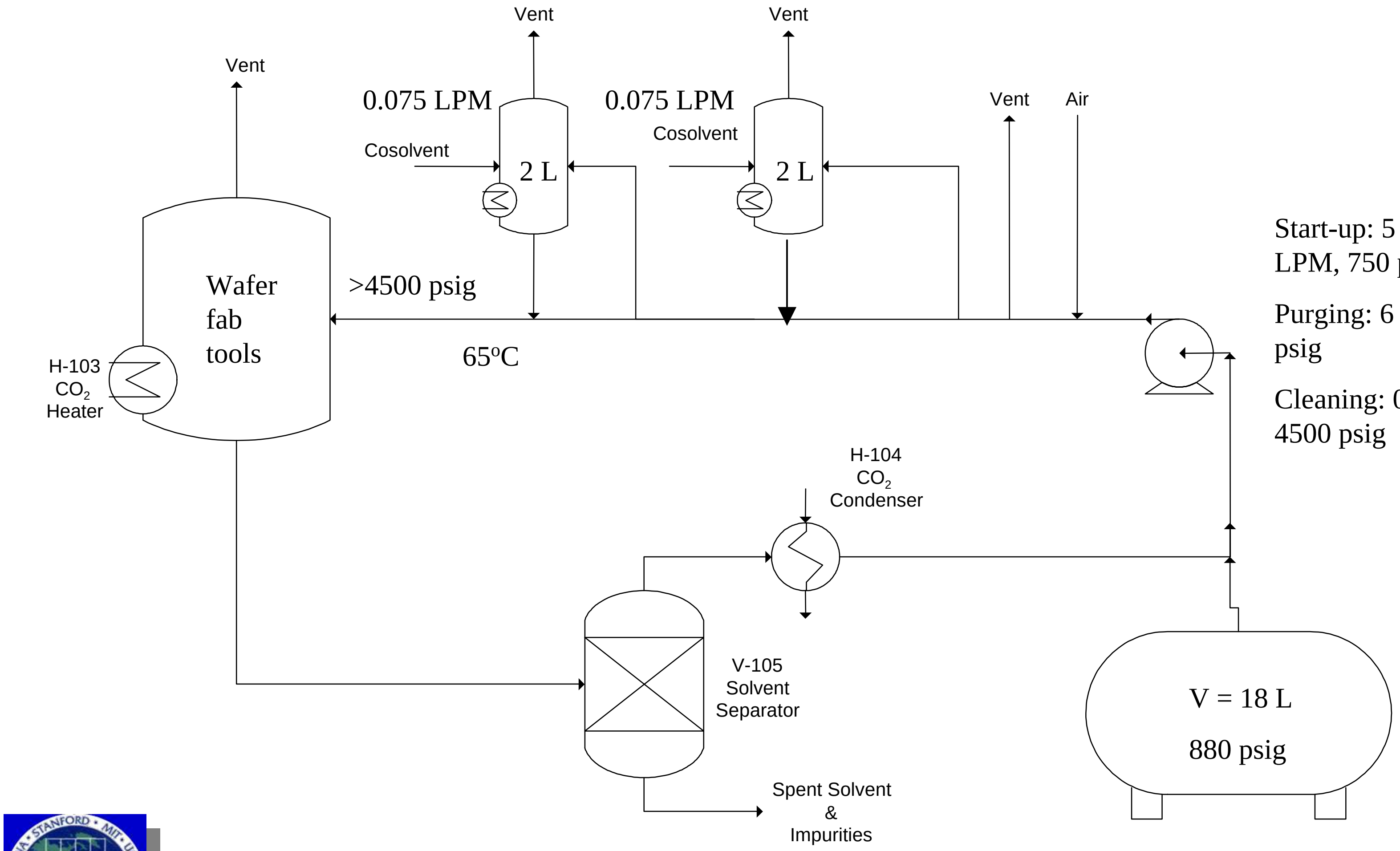


Heat transfer correlations from McCabe, *et al.* (2001)

Energy balance correlations for heats of vaporization, Felder, *et al.* (2000)



The flowsheet again with numbers and conditions



Start-up: 5 seconds, 6 LPM, 750 psig, -40°C

Purging: 6 LPM, 1500 psig

Cleaning: 0.5 LPM, 4500 psig

Assumptions Used in Calculations

Limited data for propylene carbonate heat capacities

Assumed linear function of C_p with T and expanded to T's outside of measured range

Masses of CO_2 lost per cycle

Assumed that the total tank volumes of the system would need to be purged per cleaning cycle and this CO_2 lost

Number of wafer in each CO_2 cycle

No numbers given so assumed worst case scenario of 1 per cleaning cycle

An increase in this number reduces the impacts by that amount per wafer!

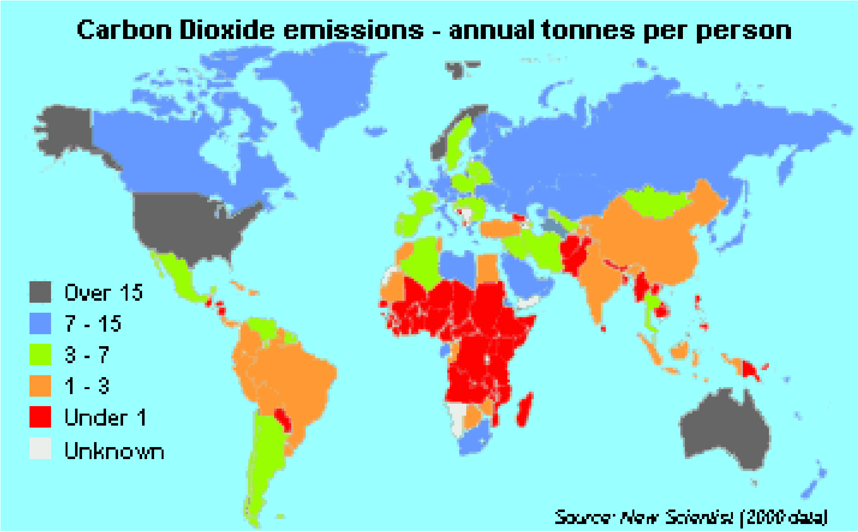
Material Balance Needs per Cycle

Per cleaning cycle, there will be some losses of CO_2 during start-up and purging.

Mass lost = 1.01 kg/cleaning cycle

There will be some propylene carbonate lost per cleaning cycle during separations unless this substance is purified from the contaminants and recycled.

Mass lost = 0.272 kg/cleaning cycle



Carbon Dioxide emissions - annual tonnes per person

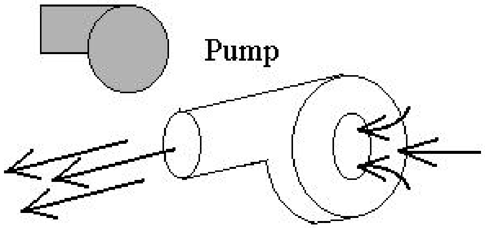
Source: New Scientist (2000 data)

May have emissions concerns if regulations on CO_2 become more stringent

Energy (kJ) Estimates for Equipment (Assume 1 cycle = 1 wafer)

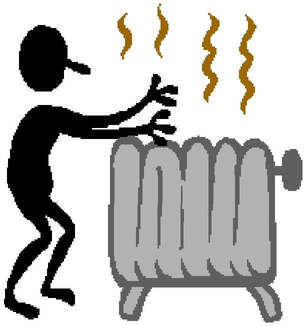
Processing Step	Piece of Equipment	Energy Duty (kJ/cycle)
Start-up	Pump	negligible
Purging	Heater	134.71
Clean and Separation	Cooler*	-151.46
	Pump	52.58
	Heater	173.70
	Separator heater	125.35
Flush	Cooler*	-97.33
	Pump	35.07
	Heater	98.57
	Separator heater	83.71
*Cooler (10^{o}C)	Refrigeration cycle	298.28

Energy Estimates for Equipment (Assume 1 cycle = 1 wafer)



Total CO_2 pumping cost per cycle = 86.75 kJ

Energy cost of mixing per cycle = 0.02 kJ



Energy cost of heating pressure chamber and cosolvent vessels = 616.04 kJ

Cooling costs = 248.79 kJ

Costs for cooling shifted to refrigeration = 298.28 kJ

Total energy costs = 1001.97 kJ per cycle

Note: did not estimate the energy requirements of separation and recovery steps of cosolvent

Recovery of PCO_3 from the waste stream could be energy intensive (not described in any patents or publications)

Largest energy costs are for heating the pressure chamber

Validation of Results So Far

Water is somewhat recyclable, but $scCO_2$ may be 100% recyclable due to ease of separations as sc conditions are removed → less energy (separation costs)

All research shows CO_2 to be 100% recyclable

One company has verified that many of our estimates are in fact close to processing numbers → assumptions are correct so far.

Some published information not available from national labs due to security concerns → cannot verify results versus actual measurements and non-patent data

A Comparison to UPW Use

A typical fabrication facility will use approximately 2,000 gal of UPW to make one eight inch wafer with about 60% of the water being used in wafer rinsing

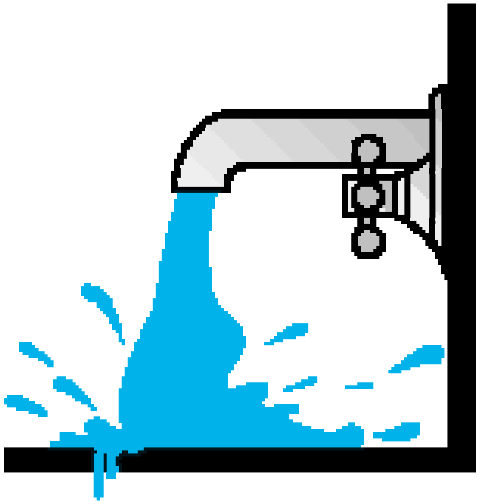
And, it takes about 46 kWh of energy to produce 1000 gal of UPW

There are approximately 130 wafer rinsing steps in semiconductor manufacturing chains based on water usage per tool

A Comparison to UPW Use: Materials

30 to 40 percent of the UPW will be sent to the sewer after rinsing.

This water may be reused internally prior to sewering, but it will still need to be replaced by fresh city water. This means that up to 480 gal (1817 kg) of water need to be provided for rinsing of each wafer processed, or **3.69 gal (13.97 kg)** per cycle per wafer .



A Comparison to UPW Use: Energy

Total Energy Requirements are 1,528 kJ/wafer/ cleaning cycle

This is an increase of 52% over the energy cost of $scCO_2$ if only one wafer can be processed at a time, but much larger than that if multiple wafers can be cleaned.

Other LCI/LCA Impacts to Quantify if Boundaries are Expanded:

Trade-offs

There are no dedicated CO_2 distribution networks like there are for water. CO_2 will need to be transported by truck → fossil fuel depletion, smog formation, greenhouse gas emissions.

Disposal of CO_2 for equipment maintenance, leaks, etc., would add to CO_2 emissions.

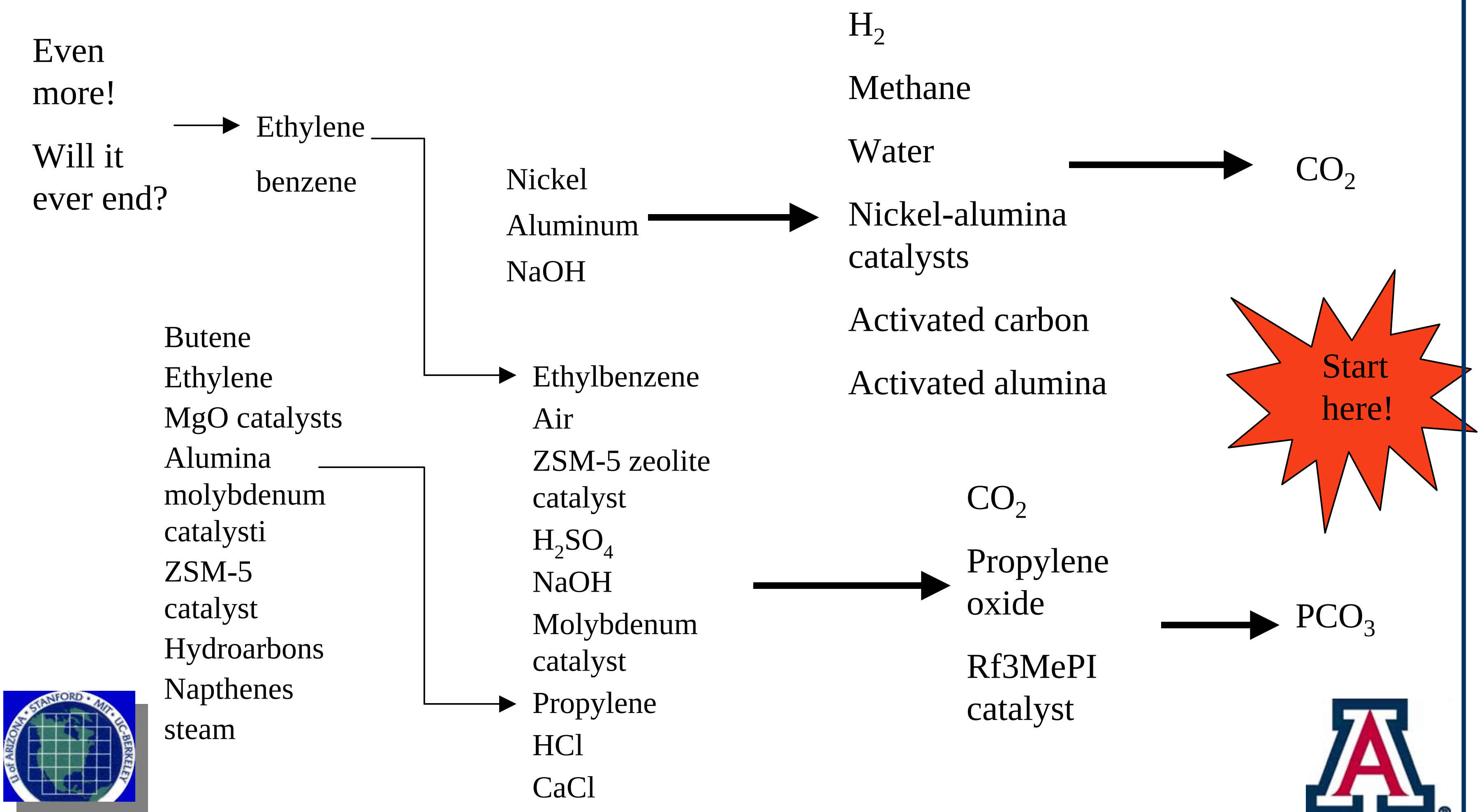
Upstream manufacturing of $scCO_2$ of this high purity may add to energy costs during production → fossil fuel depletion, greenhouse gas emissions.

Water is a resource that is being depleted rapidly in many areas where semiconductor plants are located → nonrenewable resource depletion

Need to follow-up on PCO_3 recycling and separations to make sure they are 100% and what those costs are

Future Work: Expanding Boundaries

Expand LCA back upstream to quantify overall impacts from manufacturing CO_2:



Even more!

Will it ever end?

Ethylene

benzene

Butene
Ethylene
MgO catalysts
Alumina
molybdenum
catalysti
ZSM-5
catalyst
Hydroarbons
Napthenes
steam

Nickel
Aluminum
NaOH

Ethylbenzene
Air
ZSM-5 zeolite
catalyst
H_2SO_4
NaOH
Molybdenum
catalyst
Propylene
HCl
CaCl

H_2
Methane
Water
Nickel-alumina catalysts
Activated carbon
Activated alumina

CO_2

Start here!

CO_2
Propylene oxide
Rf3MePI catalyst

PCO_3

Future Work: Cost of Ownership

The next step in making this work relevant is to complete a cost of ownership study to estimate the fixed and operating costs for the $scCO_2$ process.

Some information may be available from SC Fluids who has licensed the technology from Los Alamos National Labs.

The price of CO_2 and PCO_3 are both important to the economics since they are lost during manufacturing.

Future Work: External Decision Information Gathering

Money for large expansion of $scCO_2$ and PCO_3 use

PCO_3 is used as a reactive diluent to reduce cost in applications such as isocyanate (PMDI) wood binders / adhesives and urethane coatings / elastomers / adhesives.

A more recently discovered application for PCO_3 is in rechargeable lithium batteries. Eighty percent of a rechargeable lithium battery is the filler, PCO_3.

How much can the market bear for increases?

Optimization of $scCO_2$ process - if costs are problematic, it may be necessary to optimize the process instead of just having it workable for this application.

Vendor collaborations to address concerns can address other COO and external information concerns.

Conclusions

$scCO_2$ has many advantages over UPW use for wafer rinsing

- can recycle without contamination worries
- has lower energy costs per cleaning cycle

Some disadvantages

- CO_2 emissions during purge and start-up steps
- transportation and high purity CO_2 costs may make CO_2 unfavorable from a full LCA perspective

Acknowledgments

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