Energy Usage and Mass Balance in a Dynamic Cu CVD Cycle

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Abstract

We have previously investigated components of mass balance (reactant utilization), energy consumption (wafer heating), and manufacturing cycle time using a dynamic simulation of the Cu CVD unit process as a prototype system. The simulator is based on a physical model of the process and equipment, and captur es the essential dynamic behaviors as well as the time-integrated behaviors through the process cycle. We have since expanded and enhanced these studies to obtain a more comprehensive picture of the important factors in these metrics. We have incorporated energy costs associated with pumping equipment and other components along with the previously treated wafer heating component of energy usage in the Cu CVD process. In fact, pumping systems not only consume more energy than wafer heating and other factors, but their energy usage varies considerably depending on the details of the pump types chosen, both in average power through the process cycle and in dynamic power fluctuations that occur during key transitions of the process cycle. Accordingly, there may be real ESH benefit in working closely with component supplies to choose components that are adequate to the product performance and manufacturing cost metrics, and at the same time beneficial to ESH metrics. In addressing mass balance from the perspective of reactant utilization and its relation to process cycle time as a function of pressure, temperature, and gas flow rates, both win-win and trade-off situations emerge. The former is easy to treat, but a more careful analysis methodology is needed to manage tradeoff situations. We have begun to outline an approach to this challenge which includes consideration of manufacturing cost components and also linkages to ESH impacts beyond the factory.

Overview

1) **Understanding and enhancing the ESH aspects of semiconductor manufacturing requires impact assessment for materials mass balance and energy usage.**

2) **ESH benefits can only be obtained within the context consistent with the requirements of technology performance and manufacturing competitiveness.**

3) **Physically-grounded modeling and simulation is a valuable platform for evaluating how ESH, manufacturing, and technology metrics together change under situations of evolutionary or radical process change.**

4) **We are employing physics-based dynamic simulators to extract these multiple metrics as a function of process recipes and equipment design.**

Status

- **Cu CVD was chosen as a unit process testbed for assessment of ESH metrics within context of manufacturing and performance measures.**

- **Previous results:**
  - ***Mass balance on Cu precursor utilization and process cycle time, revealing some win-win situations for these metrics, along with tradeoff situations.***
  - ***Energy consumption associated with wafer heating, showing win-win situation for higher temperature (power) to achieve shorter process cycles and correspondingly lower energy consumption***

- **Current results:**
  - ***Energy consumption analysis expanded to include multiple terms, identifying pumping system energy as the dominant contribution and the existence of significant differences in power requirements for different types of pumps***
  - ***Further evaluation of tradeoff situations in mass balance, seeking means to combine disparate ESH metrics on the bases of economics and environment***

Modeling and Simulation

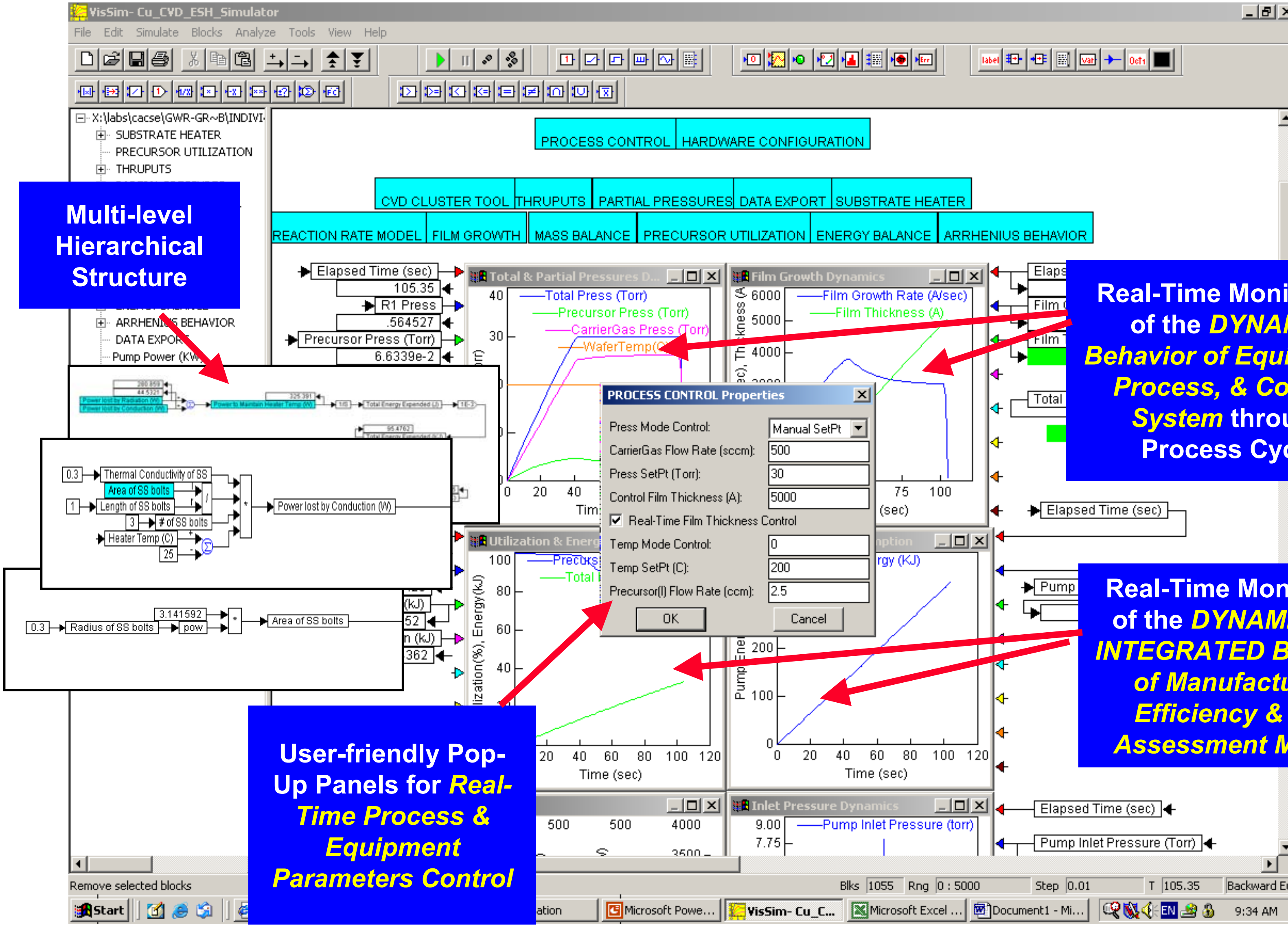
BASIC PREMISE:

Exploit modeling and simulation to reveal trends and insight into complex system behavior

Use modeling/simulation results to prioritize and justify real experiments to determine if predicted improvements can be realized

- **Build models and simulations which combine:**
  - *Physics, chemistry, etc. wherever possible*
  - *Empirical behavior (black box) wherever needed to complete a systems-level picture*
  - *Reduced-order models to enable construction of larger-scale systems models involving multiple complex components*
- **Extract both dynamic (transient) phenomena and time-integrated metrics**
- **Use virtual experiments (models & simulations) to investigate qualitative and semi-quantitative systems-level behavior to identify opportunities for potentially significant improvement**
- **Where significant improvement seems possible, carry out real experiments for optimization and model validation/improvement**

Dynamic Simulator



Multi-level Hierarchical Structure

Real-Time Monitoring of the *DYNAMIC Behavior of Equipment, Process, & Control System* through Process Cycle

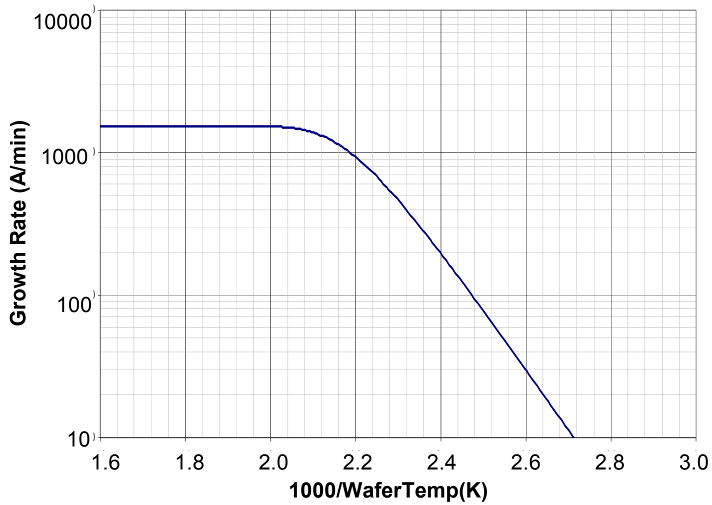
Real-Time Monitoring of the *DYNAMIC and INTEGRATED Behavior of Manufacturing Efficiency & ESH Assessment Metrics*

User-friendly Pop-Up Panels for *Real-Time Process & Equipment Parameters Control*

Blanket Cu CVD Process

$2\ Cu^{I}(hfac)(tmvs) \rightarrow Cu^{0} + Cu^{II}(hfac)_2 + 2(tmvs)$

Available as Schumacher CupraSelect™
Liquid at R.T.
tmvs = trimethylvinylsilane $C_5H_{12}Si$
hfac = hexafluoroacetylacetonate dihydrate $C_3HF_6O_2$
➔ Delivered to the showerhead using DLI system.



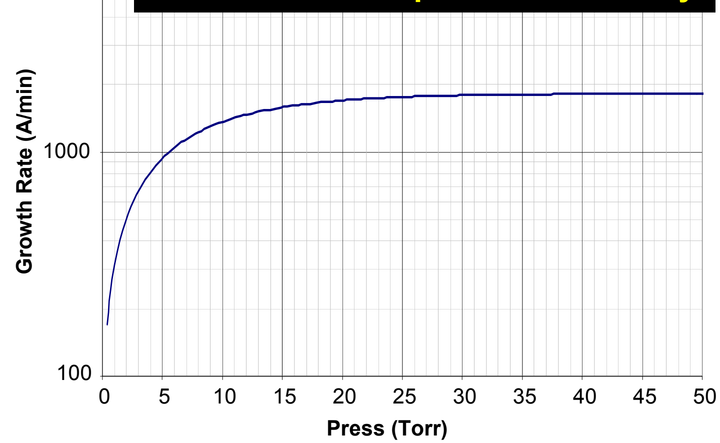
ARRHENIUS CURVE SIMULATION **– Effective Rate of Rxn composed of Transport-limited & SurfaceRxn-limited Regimes**

<u>PROCESS CONDITIONS FOR SIMULATION</u>

Substrate Temp 150 - 250°C (180 - 200°C)
Vaporizer, Gas Lines and Chamber at 60-65°C.
Ar/He CarrierGas Flow 50 – 500 sccm (100 sccm)

<u>CupraSelect™ Liquid Flow</u>
0.1 – 0.25 cc/min (for seed 200 - 500 A)
up to 2.5 cc/min (for fill 200 - 500 nm)

simulation model incorporates details of known process chemistry



ARRHENIUS PRESSURE CURVE SIMULATION **– Pressure-dependence of Growth Rate at fixed Temp & Flow Rate**

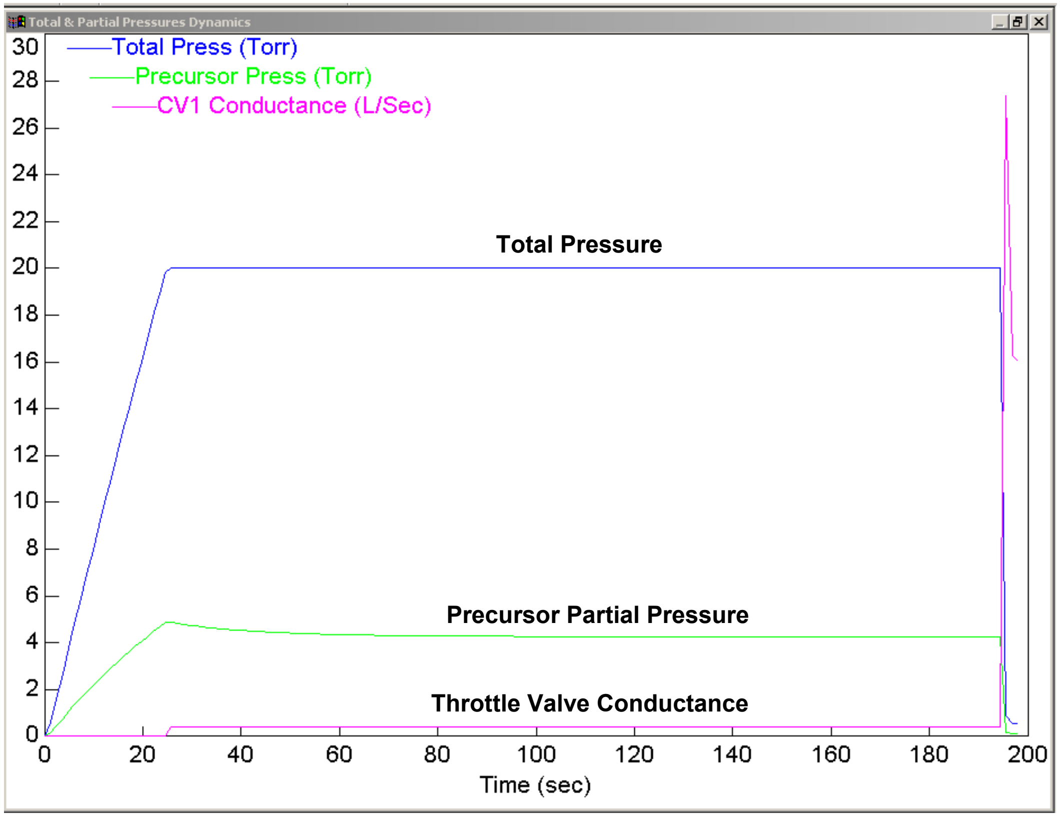
Dynamic Behavior

Dynamic behavior of process and equipment through the process cycle is revealed by simulator, e.g.,

- Total chamber pressure
- Precursor partial-pressure
- Throttle valve conductance

Detailed physical response has more complex time-dependence than might be expected from nominal process recipe, e.g.,

- Precursor partial pressure shows dynamic effects associated with changing residence time in reactor



Dynamic Behavior

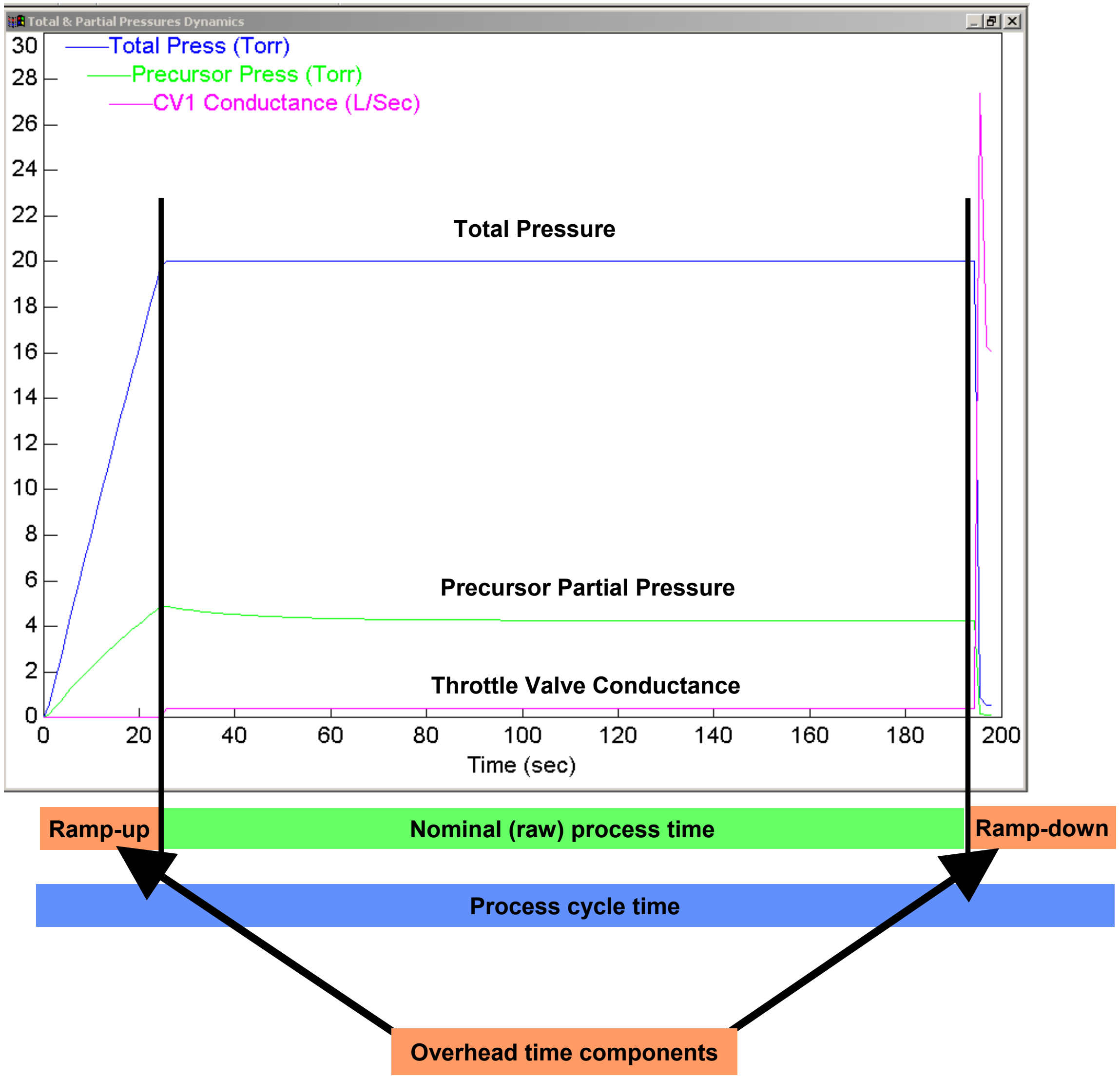
Overhead time

- *Ramp-up and ramp-down time*
- *Could include other factors (e.g., wafer exchange time)*

Cycle time = nominal process time + overhead time

Manufacturing and ESH metrics depend on full process cycle time

- *Motivation for simulation of time-integrated metrics*



Time-Integrated Behavior

Signals integrated through complexity of the detailed process cycle determine environmental and manufacturing metrics (e.g., reactant consumption)

Desired process conditions for high reactant utilization in general:

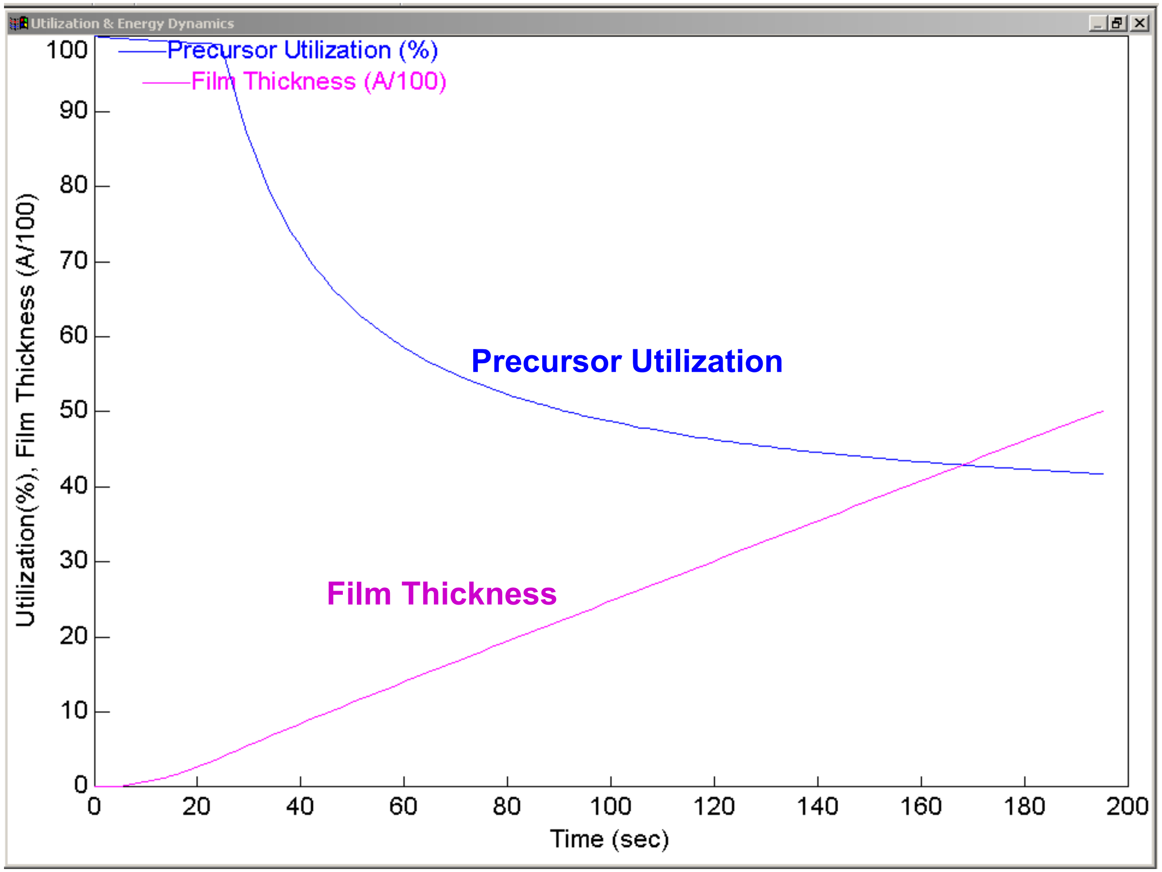
High Total Press, High Reactant Partial Press, High Temp, Low Flow Rate

⇩

Increase Residence Time
High Growth Rate

⇩

High Precursor Utilization



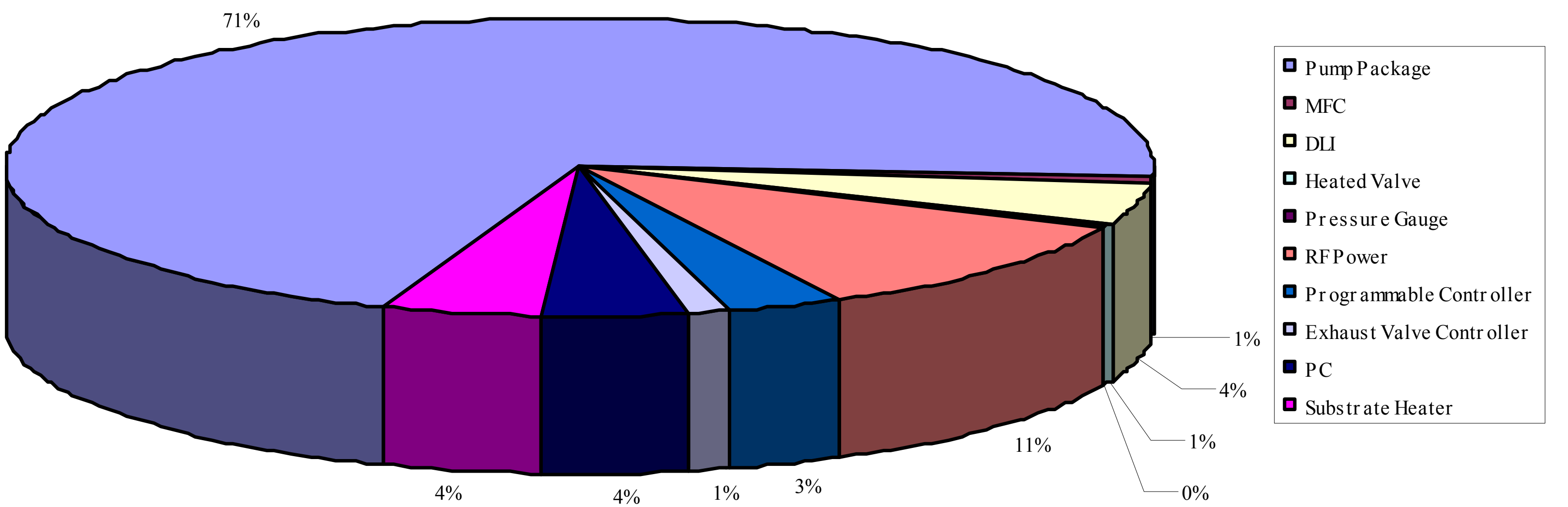
Precursor utilization (%) = # of moles of precursor reacted / # moles input

Power Sources - Pareto Analysis

Sources of Energy Use:

Substrate Heater, **Process Pumps**, **Process Chamber, Vaporizer & Gas Lines Heating, DLI System Pumps, Pre-Heated Precursor, Process & Equipment Control Units, PC's, etc.**

Sources of Energy Use	Power (KW) per Unit
Pump Package	3.26
MFC	0.0267
DLI	0.2
Heated Valve	0.03
Pressure Gauge	0.005
RF Power	0.5
Programmable Controller	0.15
Exhaust Valve Controller	0.05
PC	0.2
Substrate Heater	0.2



Data sources: (1) Leybold Vacuum Product Inc. (2) MKS Instrument (3) Ulvac Technologies Inc.

Power and Energy

Substrate Heater:

Heater kept at high temp at all times

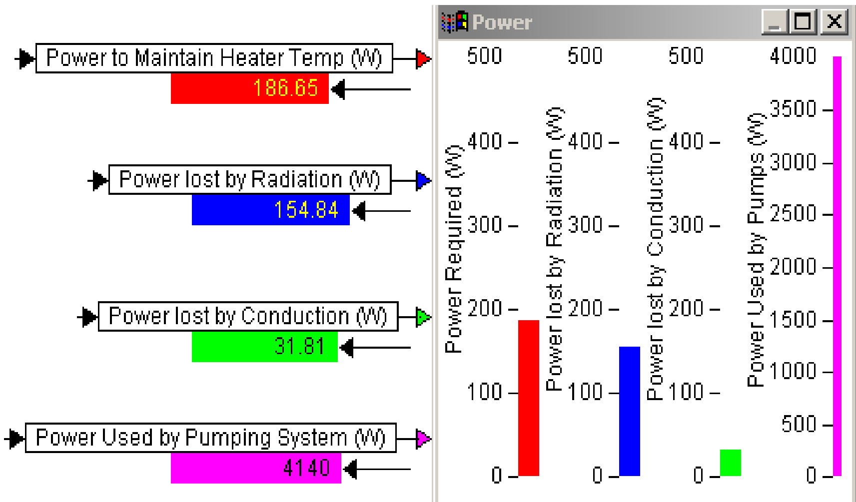
Radiative Heat Loss ~ $(T_2)^4$

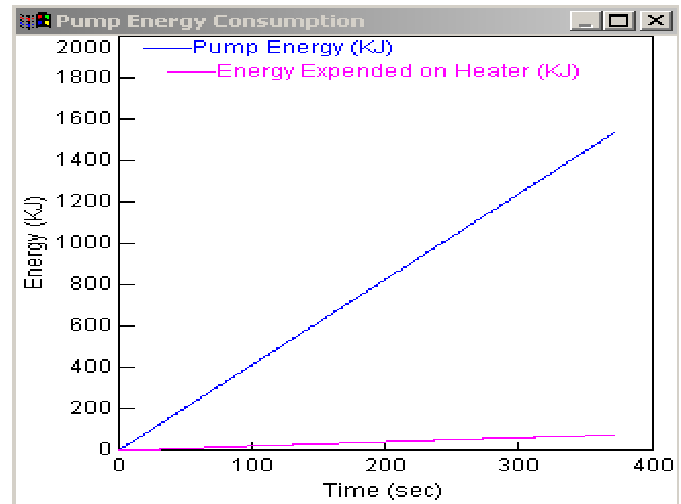
Conductive Heat Loss ~ $(T_2\text{-}T_1)$

Pump Package:

Pumps kept running at all times → significant energy consumption

Pump power is a function of pump inlet pressure → power difference during process time and pump-out time

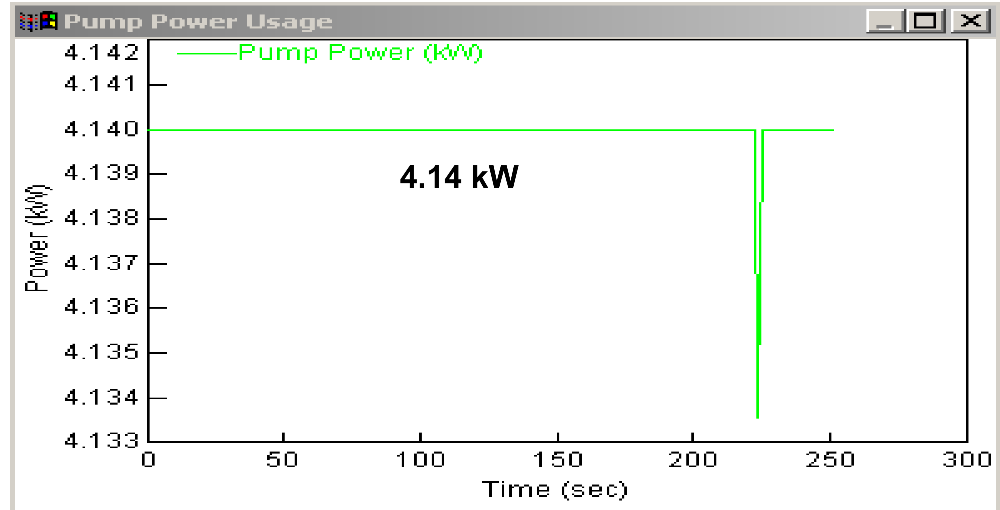


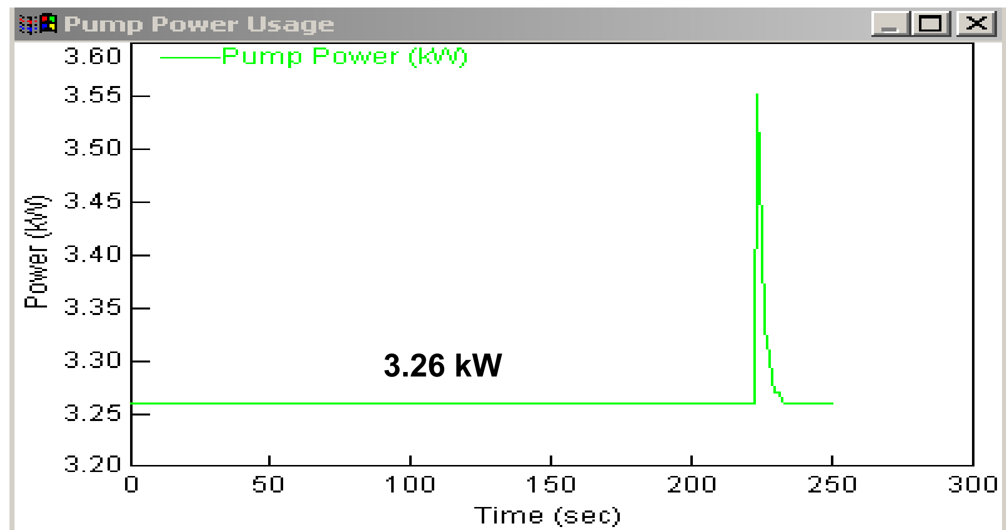


Pump system is the dominant energy consumption source in Cu CVD process

Pump System
Power & Energy Analysis

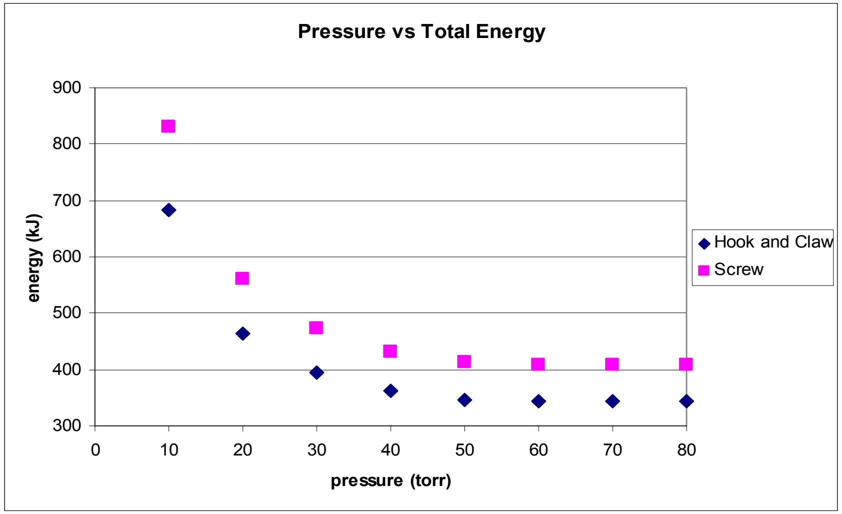
- Pump power nearly constant through entire process cycle
- Significant difference in power consumption for different pump types (25%)
- Different transient behavior for different pump types during end-of-process pump-out
- Integrated energy of transient is small cf. average power usage integrated through process cycle
- Choose energy-efficient pump on basis of average power consumption

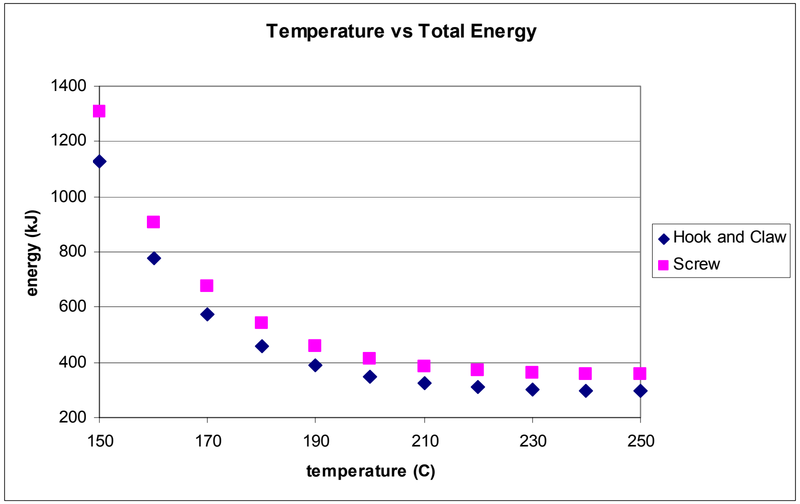


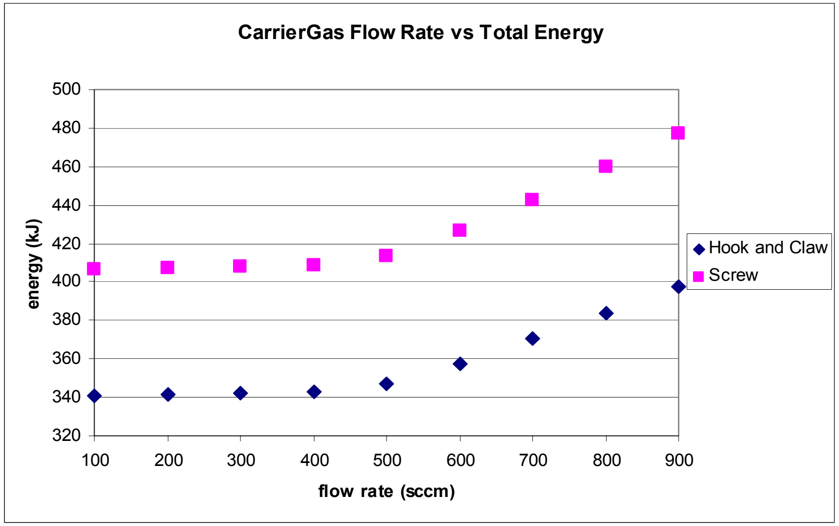


Pump data from Leybold Vacuum Product Inc.

Optimizing Energy Consumption in Cu CVD







Energy usage scales directly with cycle time in our example:

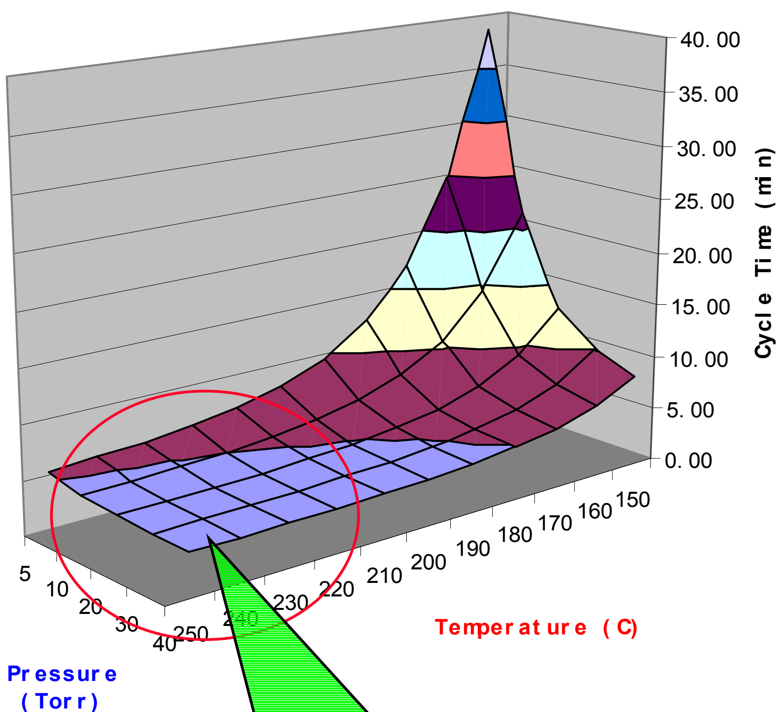
To minimize energy usage, minimize cycle time by using high temperature and pressure

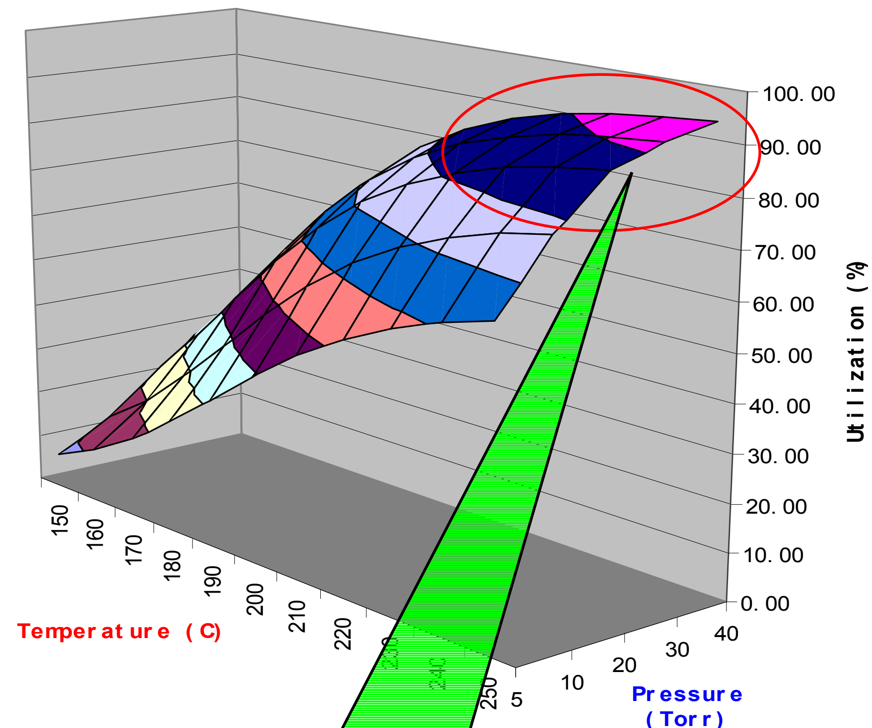
Too high flow rate will also increase the energy usage:

Limit flow rate retain short process cycle

Energy optimization in Cu CVD:
Choose energy-efficient pump system
Maintain short process cycle
(win-win situation with manufacturing throughput)

Mass Balance Optimization: Cycle Time & Reactant Utilization



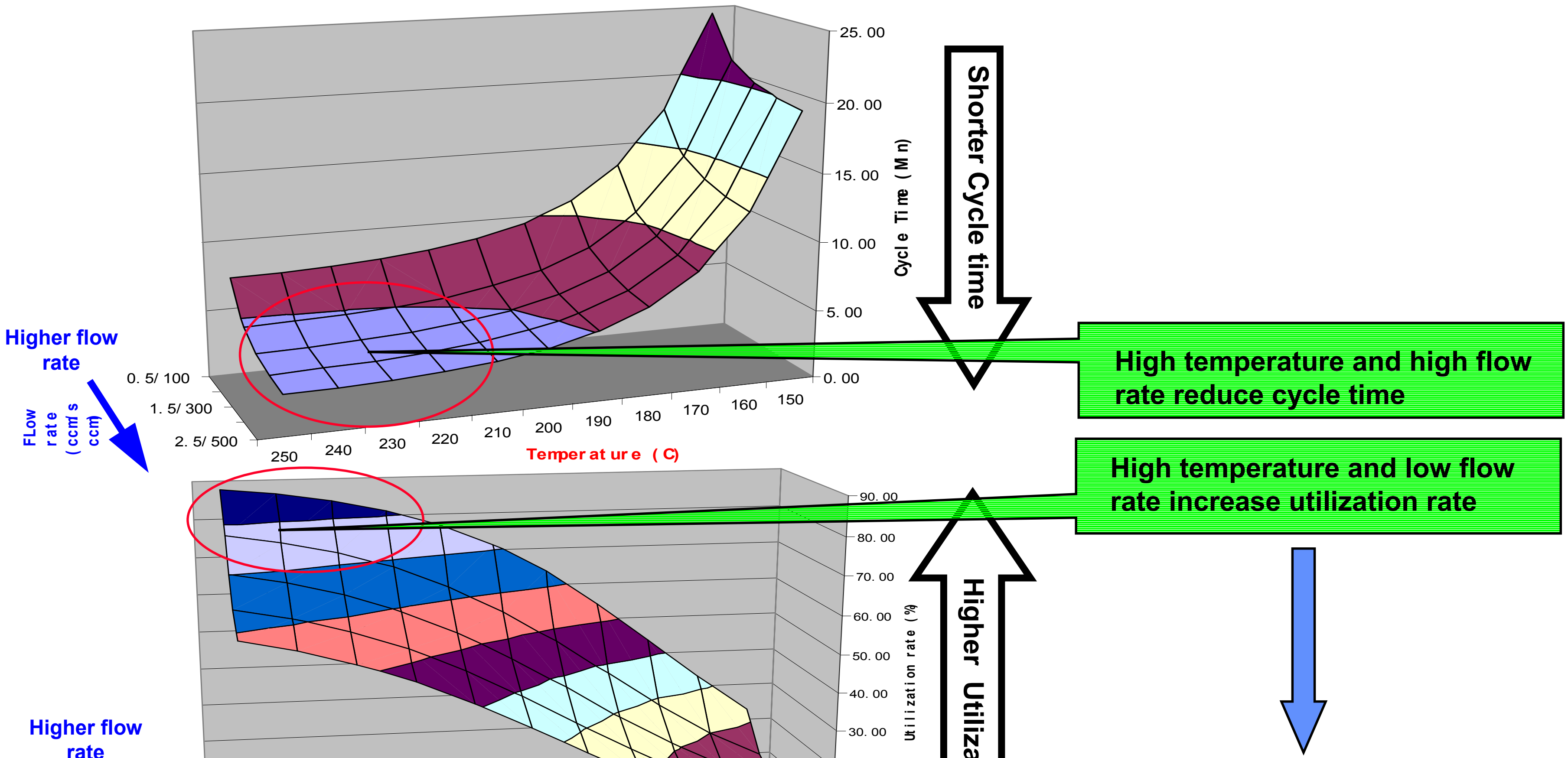


High temperature & High pressure reduce cycle time

High temperature & High pressure increase utilization efficiency

win-win region for cycle time and utilization

Mass Balance Optimization: Cycle Time & Reactant Utilization



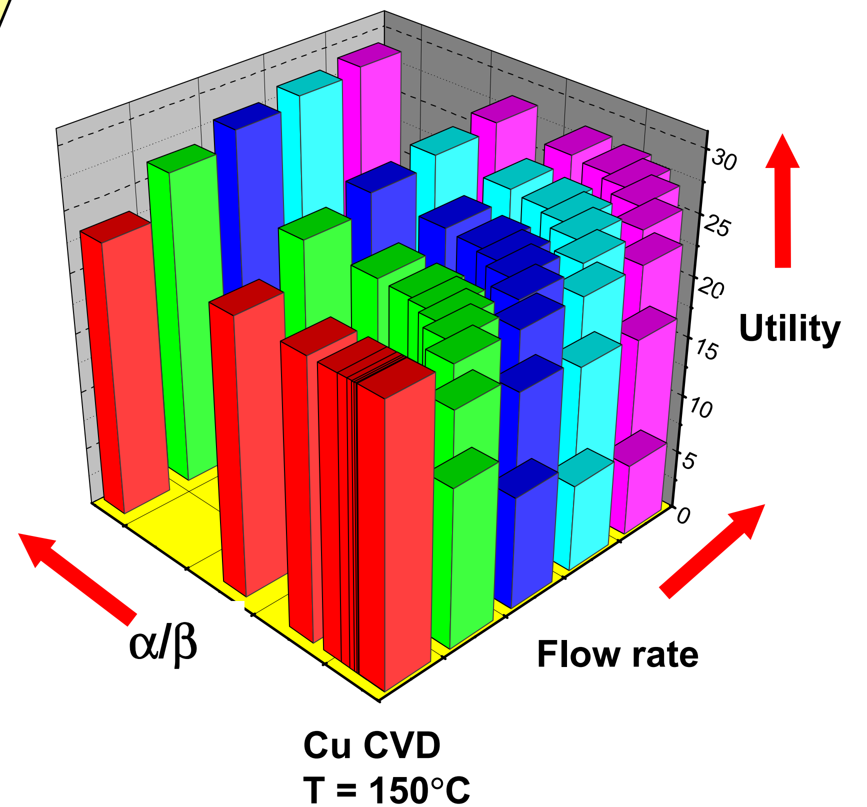
Flow rate forces tradeoff between cycle time and utilization rate

Utility Function Analysis

- **Tradeoff situations pose a common and substantial challenge**
  - *Here, increasing flow rate reduces materials utilization while improving cycle time*
- **QUESTION: how do we combine these very dissimilar metrics?**
- **ANSWER: systems engineering tells us to define a utility function that depends on the different metrics, e.g. the example in the expression above**

$$Value = \alpha \times \frac{1}{CycleTime} + \beta \times Utilization$$

- **Calculate Utility for various α/β**



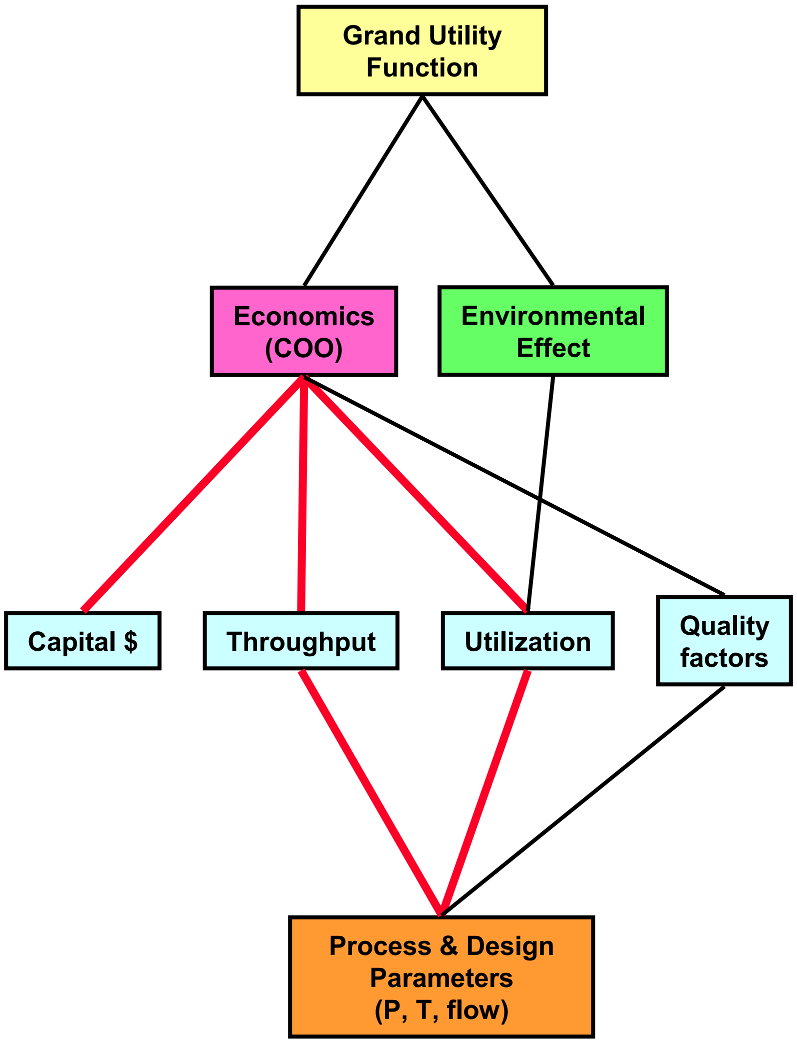
- **Note that Utility is optimized at low flow rate for small α/β (where utilization is primary determinant of Utility), and correspondingly for the other case**
- **<u>Defining a meaningful Utility function is a major challenge</u>**

Utility Function for ESH Assessment

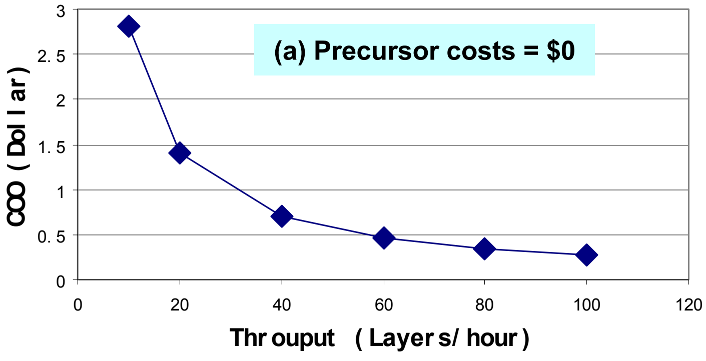
- **Utility functions for ESH impact assessment should include:**
  - *Economic factors, determined as COO*
  - *Environmental factors, addressing in-fab and direct upstream and downstream consequences of in-fab practice*

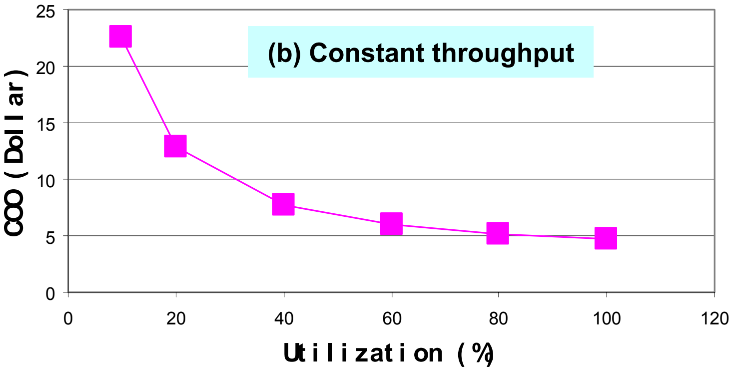
- **These link to UCB and MIT activities**
  - *EnV-S analysis of ESH COO*
  - *MIT assessment of upstream multipliers on in-fab process choices*

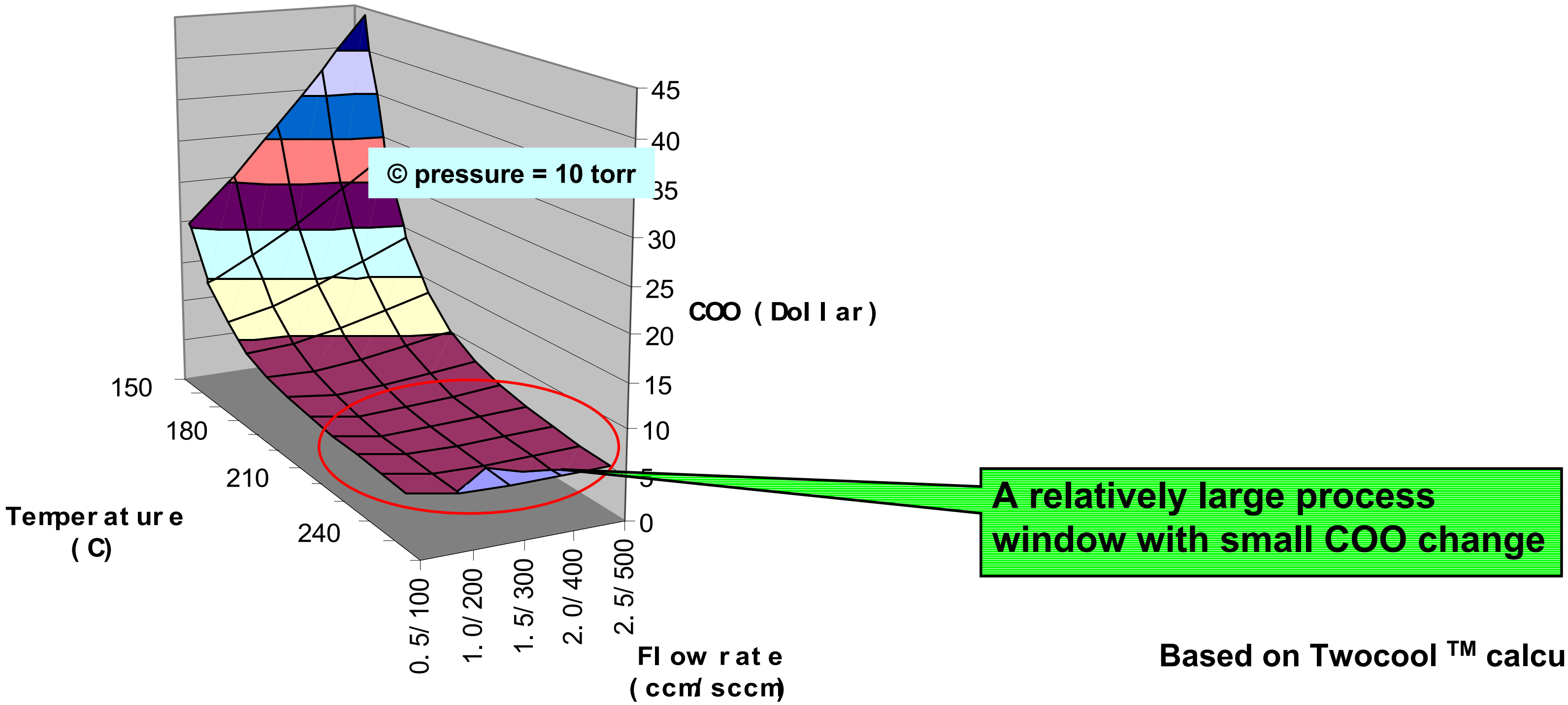
- **Use highly reduced Cost-of-Ownership model for Cu CVD process to begin such an evaluation at the unit process level**



Utility Function Analysis - COO







Based on Twocool TM calculation

Conclusions

- **Expanded analysis for Cu CVD shows that pump system configuration is the dominant component of energy consumption**
  - *Opportunity for improvements in concert with component suppliers*
  - *Thoroughness of Pareto analysis is essential*
  - *(Not all technical factors in pump choice yet addressed)*

- **Evaluation of mass balance reveals clear tradeoffs between competing manufacturing and ESH metrics**
  - *Assume that such tradeoffs are common situation*
  - *Must deal with constructing sensible utility functions*

- **Economics and environmental perspectives drive different components of ESH assessment**
  - *Economics (COO) in the fab*
  - *Environmental coupling to mass and energy consequences directly relating to in-fab practice*

- **Initial ESH COO evaluation for Cu CVD indicates relatively broad process parameter regime with minimized COO**