Integrating Life Cycle Analysis (LCA) with Process Modeling

Yue (Nina) Chen[1], Gregory J. McRae[1], Karen K. Gleason[1]*

[1] *Massachusetts Institute of Technology, Cambridge, MA 02139, USA*

* *Corresponding Author, mcrae@mit.edu, 1-617-253-6564*

Abstract

One of the main obstacles of directing process design/optimization with LCA is the disconnect between the two despite significant overlapping of information needed for both analyses. To bridge this gap, an integrated system with a process modeling environment, an LCA model, an uncertainty analysis tool, and chemical databases are proposed. The process modeling environment allows easy accumulation of process models that can be used across the academia and the industry. A case study of the chamber cleaning process using existing commercial software illustrated the system. The global warming potentials (GWP) induced by different etch rate requirements were compared. The physical and chemical databases that are part of the commercial program Aspen Plus® ease the data collection effort in process modeling. These databases and the LCA database need to be connected by sharing the same primary key.

1 Introduction

Competition requires companies to make decisions that satisfy multiple criteria. Considering profitability alone is no longer sufficient. Ignoring environmental considerations will not only expose a company to potential regulatory costs, but also damaged public image, both of which in turn have negative effect on the economic wellbeing of companies. Several examples have also proven that treating environmental consideration as an objective rather than a constraint in decision-making contributes positively to the profitability [11,15].

One of the major obstacles for integrating LCA into process design and optimization is that these two are segregated, despite much overlap in data requirement. In order for the LCA to provide useful and actionable suggestions on process design and optimization, the effects of process recipes and tool selections on life cycle impacts need to be clear. The second barrier is the limited availability of data required by environmental safety and health (ESH) evaluations. Their quality also varies considerably. For example, the typical uncertainties in toxicity (cancer) indicators for discharge to water range from 2 to 3 orders of magnitude, while those in toxicity (non-cancer) indicators range from 3 to 6 orders of magnitude [7]. This requires uncertainty to be directly addressed in the analysis.

The process modeling in most of the existing LCA studies are ad hoc. Researchers use various programs and languages to develop process models. Existing LCA software does not have extensive physical and chemical databases, nor process modules dedicated for the semiconductor industry that can be easily customized. On the other hand, existing process modeling software does not have extensive life cycle information, nor environmental/health exposure and impact data. Without a uniform modeling environment, models built by one researcher are hard to be used by other researchers or the industry.

This paper shows a system consisting of an LCA modeling environment, a process modeling environment, chemical/physical databases, LCA databases, and an uncertainty analysis tool. A relationship diagram of the system is shown in Figure 1.

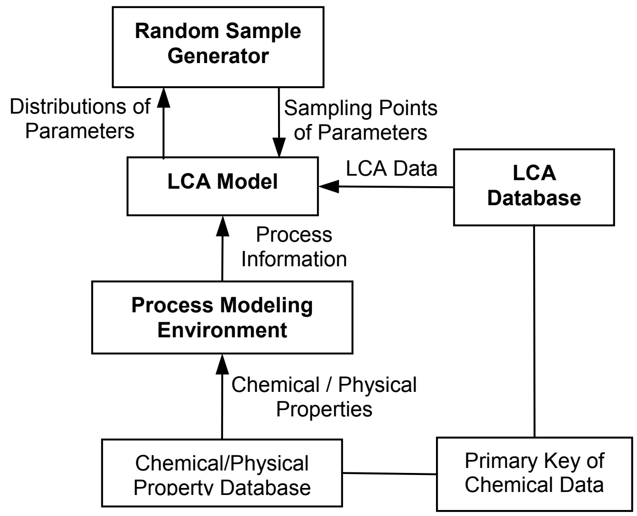

Figure 1: Integration of Software for LCA and Process Modeling

As an example, the system is realized by existing commercial software. The software used are: Aspen Plus® [3] for process modeling, Microsoft® Excel 2002 for LCA modeling, Microsoft® Access 2002 for LCA database, and @Risk® [18] for Monte Carlo simulations. Programs are connected through Visual Basic to perform a process model-driven LCA. The advantages of this integrated system are:

1. Reduced cost and time for developing a process modeling environment that is compatible with LCA from scratch.

2. It allows uncertainty analysis on both the LCA models and process models. The importance of including uncertainty analysis has gradually gained recognition in the LCA community due to the large uncertainty in the LCA data [2,14,19,20].

2 Case Study

A case study is used here to illustrate the integrated system. The system under study is a chamber cleaning process with a plasma generator, a chemical vapor deposition (CVD) chamber, and the downstream treatment system, which consists of a burner and a scrubber. The chamber cleaning process is widely used in the fab to remove the film on the chamber wall, which forms during the CVD step. This removal is necessary to reduce the particle contamination in the following steps. In the past, perfluorocompounds (PFCs) have been used to convert silicon in the film into volatile SiF4, which can then be pumped out of the chamber. Due to the high GWP of the PFCs, the World Semiconductor Council has agreed to a 10% reduction in global-warming PFC emissions by 2010, with a 1995 baseline [1]. Since then, the semiconductor industry has investigated several methods to achieve this goal. Using NF3 to substitute for C2F6 is one of them. Even though NF3 is still a global warming gas, it has a very high disassociation rate in the plasma and higher gas utilization ratio (~99%) compared to carbonfluorine cleaning, thus leaving little NF3 in the exhaust. Other exhausts from the cleaning include SiF4, F2, N2, and O2, which are not global warming gases.

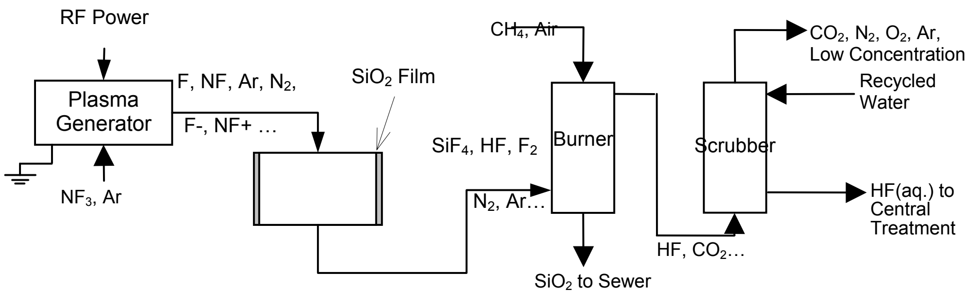

Fig 2. Schematic Picture of NF_3 Chamber Cleaning Process

2.1 Chamber Cleaning Process and Its Waste Treatment

The life cycle impacts of etch rate requirements during chamber cleaning are studied in this example. The schematic picture of the NF_3 cleaning process is shown in Figure 2. The process is to clean out 10 μm of SiO_2 film in a 300 mm wafer chamber. The plasma generator was modeled as a perfectly stirred tank reactor (PSTR) in a steady state. The number of possible reactions inside the plasma can be up to 200 [17]. The reactions considered in this work are the main reactions, i.e. the breaking down of the cleaning gases. The reactions considered for the NF_3 cleaning are:

$$NF_3 + e \dashrightarrow NF_2 + F + e$$

$$k_3 = 2.06\times10^{-17} T_e^{1.7} \exp\left(-37274/T_e\right) \tag{1}$$

$$NF_2 + e \dashrightarrow NF + F + e$$

$$k_2 = 1.57\times10^{-17} T_e^{1.8} \exp\left(-27565/T_e\right) \tag{2}$$

$$NF + e \dashrightarrow N + F + e$$

$$k_1 = 1.57\times10^{-17} T_e^{1.8} \exp\left(-27565/T_e\right) \tag{3}$$

where k_i – reaction rate coefficient for reaction i, cm^3/molecular-s,
T_e – electron temperature, K.

The chamber was modeled as a PSTR as well given its lower gas density. The etch rate of SiO_2 was correlated to the n_F and the surface temperature in an Arrehenuis form based on experimental data [12]:

$$r = (8.97 \pm 0.82)\times10^{-13} n_F T_s^{1/2} \exp\left(-0.163eV/kT_s\right) \tag{4}$$

where r – etch rate, Å/min,
eV – energy of an electron, 1.6E-19 J,
k – Boltzmann constant,1.38E-23 $m^2kgs^{-2}K^{-1}$,
T_s – surface temperature, K.

In the pipe that connects the chamber and the burner, most of the fluorine radicals recombine to form F_2.

The burner uses natural gas and air to convert unreacted cleaning gas, F_2, and SiF_4 into HF. A cyclone separates the solid SiO_2 into a sewer drain. The remaining gas goes into a counter-current scrubber. It uses recycled water from the fab to scrub HF from gas phase into the aqueous phase. The aqueous phase is then sent to the central treatment where HF is precipitated to CaF_2 by $Ca(OH)_2$.

2.2 Modeling of Chamber Cleaning Process Using Integrated System

Models of the steps described in the previous section were built in Aspen Plus®. Aspen Plus® is commonly used by the chemical industry in process design. It provides an integrated flowsheeting environment for sequential-modular, equation-oriented simulation and optimization, data reconciliation, parameter estimation and optimization [4]. The flowsheet of the chamber cleaning case is shown in Figure 3. In the actual process, SiO2 is inside the chamber before the etching starts. However, due to limitations in Aspen Plus, the model represents the SiO_2 as continuously fed into the chamber. The flow rate of SiO_2 in the model is equal to the etch rate in moles per second for real situations. The imbedded physical and chemical databases in Aspen Plus were used with the specified reactions and conditions to determine the material and energy balances for some of the unit operations. For other unit operations, design requirements were specified, such as the etch rate of the SiO_2 film. Inlet conditions were then calculated from these specifications.
To show how the changes in etch rates affect the life cycle impacts, a range of etch rates was selected. Different etch rates were achieved by varying the NF_3 flow rates while keeping the plasma power, the pressures and temperatures in the generator and the chamber, and the flow rates of other gases constant. The NF_3 flow rates and the water usages to scrub the HF to 10 ppm were calculated by Aspen Plus®. The former was then fed into the PIO-LCA model. The histogram of the ten life cycle impacts were generated by the LCA model in combination with the Monte Carlo simulations ran in @Risk®. Visual Basic macros were used to connect the programs and automate the simulations.

A Process-Product Input Output LCA (PIO-LCA) with supporting database [7-9] was used for the life cycle modeling. The set of indicators follow Eco-Indicator 99 [13]. It is to be noted that most of the parameters in the PIO-LCA model have probability distributions functions, which quantify the uncertainty in the data. The upstream inventory for the NF_3 cleaning case only included the energy usage in the production of NF_3, NH_3, and HF, with a rather complete inventory of energy generation. The energy usage of the processes were from [10,16]. These factors are modeled as normal distributions whose standard deviations are 20% of the mean values. The material and energy usage and emissions of the two cleaning processes were used as inputs for the PIO-LCA model.

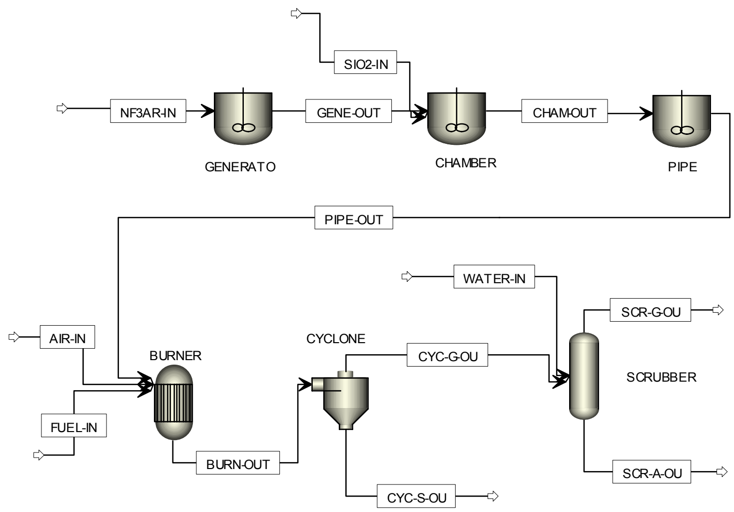

Figure 3. Aspen Plus Flow Sheet of Chamber Cleaning Process with Downstream Treatment

3 Results

The global warming potential is used as one example of the life cycle impacts to illustrate the effects of the changes of the etch rate requirements. Its result and the NF3 usage per clean are shown in Figure 4. It can be seen that as the etch rate increases, the NF3 needed to sustain the higher etch rate increases along with the GWP. However, the increase of the GWP is less steep than that of the NF3 usage. This is because a large portion of the GWP comes from generating energy for the plasma generator.

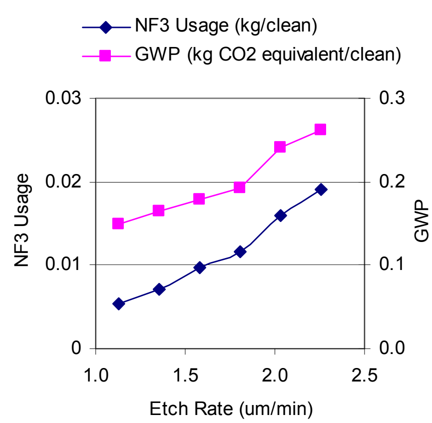

Figure 4. Changes of NF3 Usages and GWP with Changes of Etch Rates

Given the large uncertainty in the life cycle data, it is necessary to look at the uncertainty of the results. Figure 5 shows the confidence levels of the GWP at different etch rates. The confidence levels are indicated by the boxes and bars. For example, the 50% means there is less than a 50% possibility that the GWP will fall below 0.17 kg CO_2 equivalent per clean. It can be seen that the uncertainties in the GWP are significant. However, most of the uncertainty comes from emissions of power plants, the global warming potentials of emission gases, and the amount of raw materials and energy needed to produce NF_3. These factors are common to all of the scenarios studied here. Therefore, when relative GWPs are used for the comparison, the uncertainty is much smaller as the effects of these common factors cancel out. Relative GWP is defined here as

$$\text{Relative } GWP_i = GWP_{ri} / GWP_{r = 1.2\ um/min},$$

where i – number of scenario.

The result can be seen in Figure 6, which shows that all of the relative GWP is greater than one (excluding Relative $GWP_{r = 1.2\ um/min}$, which is one). Hence, in comparison of two or more processes under uncertainty, the relative ratio rather than the absolute value should be studied.

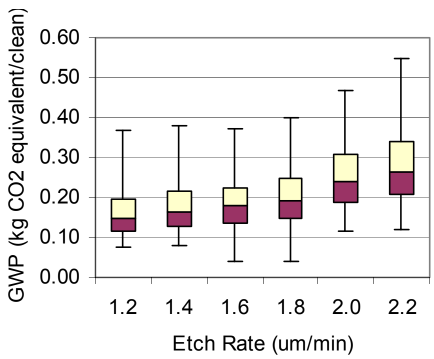

Figure 5. Comparison of GWPs of Different Etch Rates with Confidence Levels

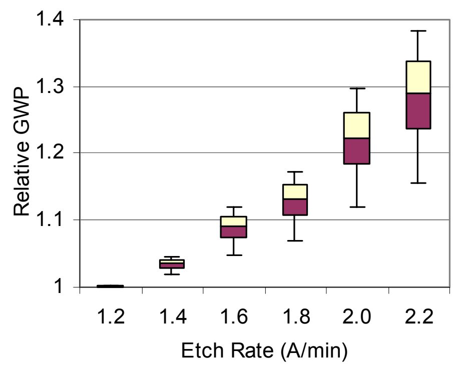

Figure 6. Comparison of Relative GWPs of Different Etch Rates with Confidence Levels

Water consumption under different etch rate requirements were also modeled. The results are shown in Figure 7. Water is used to scrubbed the HF in the gas exhaust stream to be less than 10 ppm. Facility engineers can use this information to correctly size the abatement system and plan waste water treatment capacity.

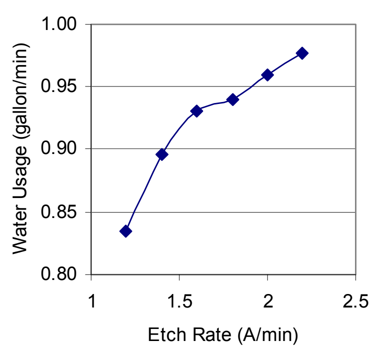

Figure 7. Changes of Water Usage with Changes of Etch Rates

4 Discussions

The set of commercial software used in this case study serves only as an example. The reason why Aspen Plus® was selected was that (a) it includes many build-in unit operations that can be customized; (b) it allows easy linkage between unit operations, therefore clusters of tools and even the whole fab can be modeled in one environment, as well as the downstream treatment processes. This makes it easier to study the impact of process designs on downstream and emissions; (c) it allows process models to be built at various hierarchy of details. Models of different detail level can be straightforwardly exchanged; (d) it also has databases of physical and chemical properties of common chemicals and estimation methods imbedded in the program. However, it is a program designed for the chemical industry. Its unit operations are not necessarily the most appropriate ones for semiconductor processes. Another program under study is TSUPREM-4 [5]. It is a computer program for simulating the processing steps used in the manufacture of silicon integrated circuits and discrete devices. It can simulate the incorporation and redistribution of impurities in a two-dimensional device [6]. It has an extensive pool of common processing steps used in the semiconductor manufacturing. Its drawback is that it does not model material and energy usages, nor emissions. However, these can be calculated from the parameters that describe the film transformation.

Aspen Plus® has extensive physical and chemical property databases. These databases provide necessary information for modeling reactions, products, and reactor conditions. These databases need to be linked to the LCA database by sharing the same primary key for the same chemical. Eventually we can imagine a highly integrated system in which once chemicals are called in process models, the system will automatically call the LCA data of these chemicals and generate the LCA model. This will greatly facilitate the use of LCA in process design and optimization.

The method and system used in this case study is generic and can be used for comparison of alternative technologies, such as NF_3 vs. C_2F_8, which is under study right now at MIT. We can imagine that over time, models of unit operations will be accumulated. These models can help both process and facility engineers in designing the processes and facility, as well as ESH personnel in understanding/predicting the impacts. More importantly, this integrated system can facilitate the communication between the parties and resolve the shortcoming of "un-actionable" of LCAs. Eventually the goal is the integration of several design criteria: technical performance, profit, and sustainability.

5 Conclusions

An integrated system of process and LCA modeling environment can be used to understand both the technical performance and the life cycle environmental impacts of processes and facility. Changes in life cycle impacts of the process recipes can be easily seen using this system. It can ease the communication between ESH engineers, process engineers, and facility engineers. A case study using existing commercial software illustrates the use of the system. To fully take advantage of existing physical/chemical and LCA databases, common primary keys need to be established for the same chemicals in different databases. More process modeling software is under study to identify the most suitable one for the integrated system.

6 Literature

[1] A Memorandum of Understanding (MOU) between the United States Environmental Protection Agency (EPA) and individual semiconductor manufacturing companies -- The PFC Emission Reduction Partnership for the Semiconductor Industry, in: (Washington, D. C., 1996).

[2] F. Ardente, M. Beccali, M. Cellura, F.A.L.C.A.D.E.: a fuzzy software for the energy and environmental balances of products, Ecological Modeling 176 (2004) 359-379.

[3] AspenTech, Aspen, in: (AspenTech Inc., Cambridge, MA, 2001).
[4] AspenTech, ReadMe.txt for AES Version 11.1 of Aspen Engineering Suite(tm) 11.1, in: (Aspen Tecch, Cambridge, MA, 2001).
[5] Avant!, TSUPREM-4, in: (Avant! Corporation, Fremont, CA, 1999).
[6] Avant!, TSUPREM-4 Manual, in: (Avant!, Fremont, CA, 1999).
[7] J.A. Cano-Ruiz, Decision Support Tools for Environmentally Conscious Chemical Process Design, Ph. D., Dept. Chem. Eng., MIT, 2000.
[8] J.A. Cano-Ruiz, New Environmental Evaluation.mdb, in: (Cambridge, MA, 2000).
[9] J.A. Cano-Ruiz, PIO-LCA macros version 3.1 revised.xls, in: (Cambridge, 2000).
[10] D.G. Coronell, T.H.-L. Hsiung, J. Withers, P. Howard, Woytek, J. Andrew, Process for nitrogen trifluoride synthesis, in, Vol. 5,637,285 (Air Products and Chemicals, Inc (Allentown, PA), US, 1996).
[11] G. Dowell, S. Hart, B. Yeung, Do Corporate Global Environmental Standards Create or Destroy Market Value?, Management Science 46 (2000) 1059-1074.
[12] D.L. Flamm, C.J. Mogab, E.R. Sklaver, Reaction of Fluorine-Atoms with SiO_2, Journal of Applied Physics 50 (1979) 6211-6213.
[13] M. Goedkoop, R. Spriensma, The Eco-Indicator 99, a damage oriented method for LCIA: Methodology Report, in: (PRe Consultant, Amersfoort, the Netherlands, 2000).
[14] B. Gonzalez, B. Adenso-Diaz, P.L. Gonzalez-Torre, A fuzzy logic approach for the impact assessment in LCA, Resources, Conservation and Recycling 00 (2002) 1-20.
[15] T.G. Gutowski, C.F. Murphy, D.T. Allen, D.J. Bauer, B. Bras, T.S. Piwonka, P.S. Sheng, J.W. Sutherland, D.L. Thurston, E.E. Wolff, WTEC Panel Report on Environmentally Benign Manufacturing, in: (International Technology Research Institute World Technology (WTEC) Division, Baltimore, MD, 2001) 31-32.
[16] M. Jaccaud, R. Faron, D. Devilliers, R. Romano, Ullmann's Encyclopedia of Industrial Chemistry, in, Vol. 2002 (Wiley-VCH Verlag GmbH, Weinheim, Germany, 2002).
[17] E. Meeks, S.R. Vosen, J.W. Shon, R.S. Larson, C.A. Fox, D. Buchenauer, Results from Modeling and Simulation of Chemical Downstream Etch Systems, in: (Sandia National Laboratories, Albuquerque, NM, 1996).
[18] Palisade, @Risk, in: (Palisade Corporation, Newfield, NY, 1996).
[19] A.K. Petersen, B. Solberg, Greenhouse gas emissions, life-cycle inventory and cost-efficiency of using laminated wood instead of steel construction, Environmental Science & Policy 5 (2001) 169-182.
[20] B. Steen, On uncertainty and sensitivity of LCA-based priority setting, Journal of Cleaner Production 5 (1997) 255-262.