2006-1009: EXPERIENTIAL LEARNING OF DESIGN OF EXPERIMENTS USING A VIRTUAL CVD REACTOR

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Experiential Learning of Design of Experiments
Using a *Virtual CVD* Reactor

Abstract
Presently there is a need for more effective ways to integrate statistical methodologies such as Design of Experiments (DOE) into the engineering curriculum. We have developed a virtual chemical vapor deposition (CVD) reactor based on a numerical simulation where students learn and then actually apply DOE. Associated educational materials are also being developed. The simulation of the *Virtual CVD* reactor is based on fundamental principles of mass transfer and chemical reaction, obscured by added "noise." However, rather than having access to the entire output of model, the film thicknesses are given to students only at the select points within the wafer and from wafer to wafer that they have decided to "measure". This package is all housed within a three-dimensional (3D) graphical user interface where students are placed in a simulated clean room environment. Student assessment is based not only on the ultimate reactor performance but also on the cost of experimentation.

This learning tool represents an innovative use of computers and simulation in integrating statistics into engineering education. Students are given a "capstone" experience in which they have the opportunity to synthesize engineering science and statistics principles to optimize reactor performance. Since the simulation is from first principles, students can interpret the outputs given by the DOE in terms of the chemical and physical phenomena in the system. The *Virtual CVD* reactor allows students a broader and more realistic experience in using the DOE methodology for process improvement - as if they were operating an actual industrial reactor.

The project scope also includes development and implementation of an assessment plan to evaluate the effectiveness of this tool in promoting higher order thinking skills. The Northwest Regional Educational Laboratory is providing support for the project evaluation and assessment. A five-member advisory committee consists of engineers and statisticians from academia (Oregon State University, University of Oregon) and industry (LSI Logic, Intel, WaferTech).

The *VirtualCVD* Learning Platform is available now for use in approved courses. Instructors who are interested in adopting this software into their curriculum can go to the following web page for information: http://che.oregonstate.edu/research/VirtualCVD

Motivation
Proficiency with statistical methodologies such as Design of Experiments (DOE) is an increasingly essential skill for engineers. This requires not only knowledge of statistical concepts related to DOE, but also the ability to integrate this methodology with fundamental engineering principles toward designing and understanding experiments. However, current engineering curriculums have not fully adapted to this need in the engineering industry. In the 1970s and 1980s, the absence of sound statistical methods in the engineering work place led to a crisis in US industry where a large percentage of the market share went overseas. This crisis was first reflected in the manufacture of automobiles and then in the process-oriented manufacture of integrated circuits.[1,2] Only with the industrial investment towards quality, largely through the systematic training and implementation of statistical methodologies, has the United States

regained competitiveness. Indeed, a survey of OSU ChE alumni found that statistics presented the largest discrepancy between the preparation at the university relative to the importance in employment.[3] This result is typical of curricula throughout the country.[4-7]

The most ubiquitous and powerful of these statistical techniques is Design of Experiments (DOE). DOE is a method for systematic planning and conducting experiments in which multiple input variables are systematically changed to observe changes in the outputs of a process. Historically, both science and engineering curricula have emphasized one-factor-at-a-time experiments where one variable (factor) is changed while the others are held fixed. This approach is wasteful and the results can be misleading. However, statistically designed experiments provide a more effective and efficient way to learn about and optimize a process. By combining the settings of several factors simultaneously in design arrays, it is possible to isolate the effects of each factor individually. A designed experiment usually requires fewer resources for the amount of information obtained, and the results are more precise since more measurements are used to determine the effect of a given factor. Moreover, the interactions between the factors, i.e., the effect of one factor on another can be quantified. Presently, DOE is largely taught to entry-level engineers by industry through in house training programs. Such skills are more appropriate to teach at the university where an educational approach emphasizing fundamentals could provide students with greater depth and adaptability in applying these methods. One constraint, however, is that the curriculum is full and, by in large, successful. The educational challenge then becomes how to integrate statistics-based topics such as DOE so that they compliment the existing educational curriculum and can be fit in; more effective methods are needed to allow students to integrate statistics and DOE into their engineering studies.

Numerous computer resources have been developed to reinforce knowledge and understanding of statistics. These applications have evolved from forms that are quite similar to conventional printed material to the development of interactive simulations that give students a *hands-on* learning experience of specific statistics concepts, e.g., the central limit theorem or sampling distributions.[8] In the classroom, process simulation is typically used for analysis where students are either asked to use commercial simulations, e.g., SUPREM-IV or FLOODS[9,10] or use simplified code to predict reactor performance. However, process engineers in industry rely largely on empirical techniques to develop process recipes that optimize performance. No tool is more critical in this process than DOE.

The undergraduate laboratory has been demonstrated to provide an effective means of teaching DOE through experiential learning.[11] However, lab experiments are expensive and time consuming; hence, there is a constraint on the proportion of topics in the curriculum that can realistically be introduced in the lab. University teaching labs can also be limited by their equipment capability. Ideally, a student would have a rich experience in DOE before entering senior lab, and then could reinforce it by creatively applying these methods to real measurements. Often, however, the bridge between what is taught in an engineering statistics class and what is required in the lab is weak.

In an attempt to meet the need for a "capstone" experience that integrates engineering and statistics, we have developed a virtual chemical vapor deposition (CVD) reactor based on a numerical simulation where students learn and then actually apply DOE. The *Virtual CVD*

reactor uses fundamental process simulation in a new and innovative way. Students will use the virtual reactor in exactly the same manner as they would a reactor in industry. They will be tasked with improving and optimizing reactor performance based on DOE. In completing this task, they will need to choose the parameters for each of the runs they perform and choose what measurements they want to make. Their choices have a cost associated with them so there is a realistic economic constraint. The most effective performance will be a balance between optimization of performance and cost. Not only must students learn how to apply DOE, they must also determine when their results are good enough and the reactor is ready for production.

Educational objectives
The complete experimental design process is depicted in the flowchart shown in Figure 1. The first step is to select a response/dependent variable (variables) that will provide information about the problem under study and the proposed measurement method for this response variable, including an understanding of the measurement system variability. The next step is to select the independent variables/factors to be investigated in the experiment. After the dependent and independent variables are selected, then an appropriate experimental design should be selected that will allow the experimental questions to be answered once the data is collected and analyzed. The experiment is then performed. Collecting data is a critical stage in DOE. The data are then analyzed using the appropriate statistical model insuring that attention is paid to checking the model accuracy by validating underlying assumptions associated with the model. Based on the results of the analysis, conclusions about the results and the physical meaning of these results are inferred. Finally the practical significance of the findings are determined, and recommendations for a course of action, including further experiments, are made. The intent of the *Virtual CVD* Learning Platform is to allow students to experience this process, from start to finish.

Specifically, the *Virtual CVD* reactor is an intervention designed to achieve the following educational objectives:

1. Design experiments to optimize the performance of a CVD reactor.
   o Identify key reactor inputs and determine relationship between input levels and achieved thin film uniformity.
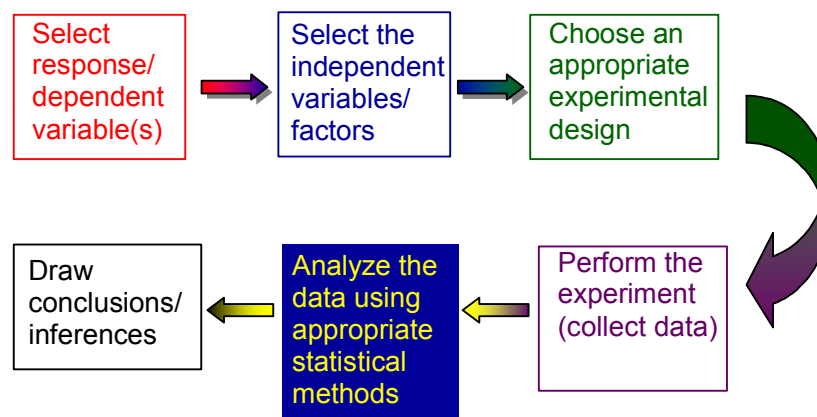
Figure 1. Overview of DOE Methodology

o Design appropriate statistical methodology to optimize the uniformity.

2. Perform virtual experiments, analyze and interpret the results.
   o Explain resulting film uniformity in terms of chemical and physical phenomena.
   o Analyze film uniformity during experimentation and iteratively modify the experimental design to account for any surprises. Explain why any adjustments in experimental design were made and their effect.

3. Synthesize and toggle between statistics and engineering science concepts while applying both in a real-world simulation.

4. Synthesize results in the form of a final written and oral report.

The *Virtual CVD* Learning Platform
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The *Virtual CVD* Learning Platform contains several components:

- Mathematical model
- 3D graphical student interface (3D client)
- Instructor web interface
- Database

The deposition of silicon nitride, Si_3N_4, films by chemical vapor deposition (CVD) was chosen as a model system to provide students experience with applying DOE. This system has sufficient complexity to warrant a methodological design approach, but also can be qualitatively considered in terms of engineering science fundamentals such as mass transport and reaction kinetics.

The deposition of silicon nitride is usually performed from ammonia and dichlorosilane (DCS). The overall reaction is given as follows:[12]

$$10NH_3(gas) + 3SiH_2Cl_2(gas) \rightarrow Si_3N_4(solid) + 6NH_4Cl(gas) + 6H_2(gas)$$

The *Virtual CVD* reactor is based on an industrial scaled vertical reactor, as illustrated in Figure 2. The process is carried out at low pressure (less than 1 torr) to enhance the diffusion of gaseous components involved in the reaction at temperatures ranging from 600°C to 800°C. The mixture of gases flows through the annular space between the wafer edges and liner while the two reactants diffuse into the space between adjacent wafers where the deposition reaction takes place. As the reactant gases flow through the annular space, their concentrations decrease due to depletion in the deposition reaction. To compensate for decreasing reactant concentrations, it is common to raise the reactor temperature towards its exit. The increased temperature increases the deposition rate. The reactor furnace typically has five heating zones used to adjust the

reaction temperature profiles. Because diffusion is the main mechanism for supplying the two reactant gases into the space between two adjacent wafers, the deposition rate around the wafer perimeter is naturally higher than that at the center. To minimize deposition thickness variations across wafers and from wafer to wafer, it is essential to determine proper feed rates of NH_3 and $SiCl_2H_2$ under proper temperature settings of individual heating zones as well as the reactor operating pressure in addition to the time for the reactor operation. Thus, there are a total of 9-10 parameters in operating a CVD reactor. It is an extremely important and difficult task for an engineer to find the optimum conditions using a minimum number of trial settings of the operating parameters. DOE is inevitably an essential tool to accomplish this task.

The simulation of the *Virtual CVD* reactor is based on a mathematical model that describes both the mass transfer and chemical reaction that take place simultaneously in a CVD reactor and predicts the local thickness of silicon nitride deposit at all radial locations on any wafer. The mathematical model is described in detail in Appendix A. Since real systems do not deterministically adhere to fundamental models, random process and measurement variation are incorporated.

The *Virtual CVD* reactor front-end is a three-dimensional (3D) graphical interface that provides the look-and-feel of a typical semiconductor manufacturing environment. From here, the students can make reactor runs, take measurements that they specify, get output data and determine the cost of their experiments. Figure 3 displays screen-shots of this interface. This front-end goes beyond simply providing a method for students to access the simulation. It also allows students to become familiar with the appearance of a cleanroom. The similarity of the 3D interface to popular video games allows this learning platform to feel familiar and non-threatening to the student.
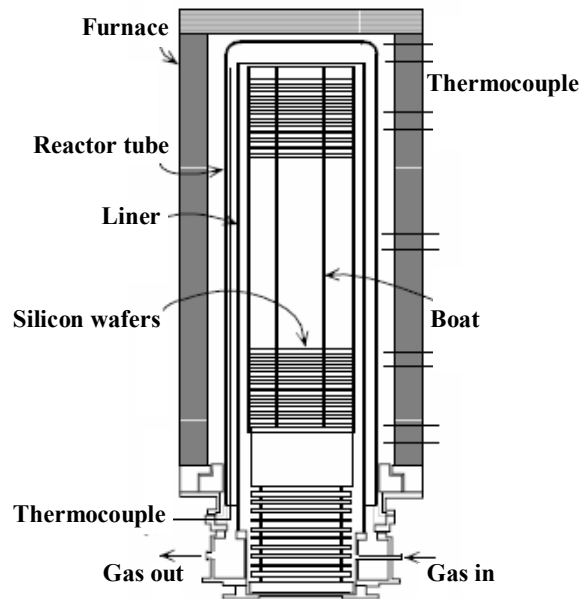
Figure 2. Schematic diagram of typical CVD reactor
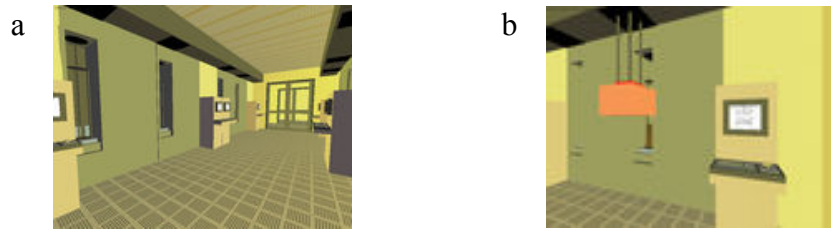
Figure 3. Screen shots of the *Virtual CVD* 3D graphical user interface a) CVD reactor bay in the virtual fab, b) wafers being loaded into a CVD furnace

To grow Si_3N_4 thin films using the *Virtual CVD* reactor, the student must typically specify 9 operating parameters. The reactor input screen is shown in Figure 4. The different temperature zones in the reactor (5 zones by default) can be independently controlled. In addition, the flow rates of ammonia and dichlorosilane feed gases, the reactor pressure and the reaction time must be chosen by the student.

After the student has run a batch of wafers through virtual reactor with a given set of input values, they have access to a virtual ellipsometer to measure the film thicknesses. They need to select the wafers they will measure and the measurement locations on those wafers as well. Figure 5 displays a view of the virtual ellipsometer console for a specific wafer. From these data, students can estimate the overall film uniformity.

The students are charged virtual money for each run and for each measurement. This feature applies a realistic cost constraint such as an engineer would experience in industry. After the student has their final optimized reactor setting, they can submit the process recipe via the 3D interface.

Figure 4. *Virtual CVD* reactor parameter inputs: these parameters must be input by the student to run the reactor.
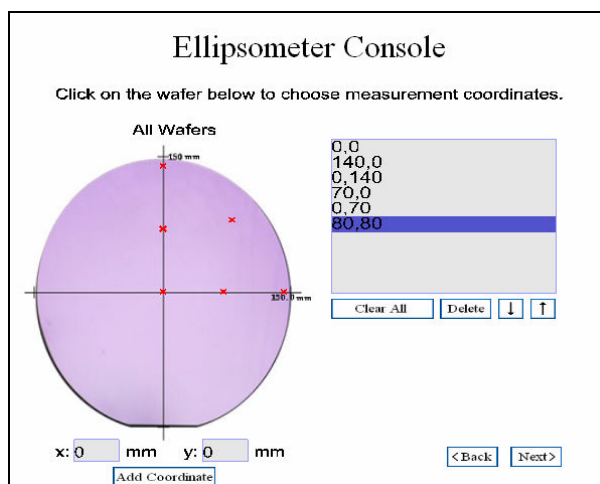
Figure 5. Selection of measurement points on a wafer. The red "x" marks indicate the positions chosen to measure. The corresponding coordinates are shown.

To implement in a course, the instructor should set-up an instructor account via the following webpage: http://che.oregonstate.edu/research/VirtualCVD/sign_up_to_use_virtualcvd.html After establishing an instructor account, the application can be personalized for use in a specific course. From the instructor's web-based interface, student accounts can be established. Students will need a username and password to run the software. If students will be working in groups, one account can be made for each group.

The instructor can customize the number of reactors available to the students, and various parameters for each reactor. However, instructors who do not wish this level of specificity can simply use the default values. Default reactor settings are shown in Figure 6. From this interface, the instructor may change the number of wafers, wafer radius, wafer spacing, and the virtual "cost" that the student is charged for making each furnace run and measurement set. The instructor can also change the number of temperature zones, the position of the thermocouple within each zone, and the "bias" associated with it. Experimental errors are added to the students' measured film thicknesses via a normal distribution with standard deviation σ. The instructor can change the parameter σ, so that smaller or larger experimental errors are observed by students.

A great benefit of the instructor interface is access to the students' interactions with the *Virtual CVD* Learning Platform. All of the student's virtual experimental activity is captured in a database and can be utilized as an assessment tool. The software makes all data for student runs and measurements available to the instructor. The instructor's web interface contains an overview page, which shows the total number of furnace runs, measurement sets, and total cost. By clicking on a student's account name, the instructor can view the student's chosen reactor parameters for each run, and the student's measurement points and resulting measured values for each measurement set. The time at which the run or measurement set was made is also shown. These data can also be exported to a Microsoft Excel spreadsheet, as individual runs, measurement sets, or as a single combined spreadsheet. An example of an instructor exporting data is shown in Figure 7.

Figure 6. Reactor parameters which may be customized by the instructor using the instructor interface.

The software design, including the student 3D student interface (3D client), instructor web interface, mathematical model and database back-end is described in Appendix B.

Implementation
A preliminary version of the *Virtual CVD* reactor was used for a pilot run in *Thin Film Materials Processing* (ChE 444/544) in Winter 2005. This version used the fundamental mathematical model associated with the *Virtual CVD* reactor. However, in this initial deployment, the user interface was HTML based rather than the 3D graphical interface that is now available. Additionally the data base was in a skeletal form and the instructors interface did not exist. The implementation is discussed below. Experience from this run has been used to enhance features. It will be used again in this elective course in Winter 2006 complete with 3D graphical interface,

Figure 7. Instructor web interface view of a student's furnace runs and measurement data.

instructors interface and enhanced database. Beginning in the 2006-2007 academic year, the *Virtual CVD* reactor will be integrated into the ChE Capstone Laboratory course (ChE 414). In this way, every ChE undergraduate at OSU will gain critical experience in the entire cycle of applying experimental design methodology prior to conducting experiments on the real equipment in the lab. The rational for integration is not content specific, i.e., microelectronics processing, but rather it is believed that the process of going through this type of design methodology will provide students with a useful experience that will effectively translate to any experimental design they may face.

The *Virtual CVD* reactor assignment used in Winter 2005 is shown in Figure 8. Eight student groups of 3-4 members completed the assignment as the final project for the course. In this assignment, the groups were asked to conduct experiments to determine a process recipe to release to high volume production. Before given access to make experimental runs, each group needed to come up with a preliminary design in the form of a "Design Strategy Memo" which was reviewed by the group and the instructor. This process ensured that the groups had a well-thought out approach before making runs (in analogy to obtaining management approval in industry). Their work during the trials could be viewed at anytime by the instructor. The final deliverables were a written report and an oral presentation as detailed in Figure 8.

A summary of the performance for each group is shown in Table 1. This table reports the overall uniformity and standard error off target for each student group. It can be seen that groups can be evaluated both by the efficacy of their process and the cost of the experimentation. The values might vary from the students' reported values because they are not limited to discrete measurement points, but rather calculated by the software to encompass an average of all the films grown without the imposed process and measurement variation. In statistical terms, the value reported to the instructor (as shown in Table 1) is the population based on the student choice of reactor parameters while that reported by the students is a sample based on their measurements. Also, the total cost of the experimentation is reported. The value is based on the number of runs and number of measurements the group has made and is also available in the student interface. The utilization of both feed gases is displayed; a critical measurement of the success of the student's effort to maximize the utilization of dichlorosilane. For each case, the value for each output of the group that has performed the best is denoted in blue.

The *Virtual CVD* Learning Platform is designed to ensure ease of transportability and adaptability to different curricular structures. In addition to the classes at OSU, the *Virtual CVD* reactor will be implemented remotely in Summer 2006 in the Semiconductor Processing and Device Characterization MS Program at the University of Oregon (UO). This internship-based program provides students with BS degrees in Physics and Chemistry background in semiconductor device physics, processing and manufacturing. While it will be implemented in a very different type of program, the *Virtual CVD* reactor will provide the same function at UO that it does at OSU - to give students hands-on experience with DOE before they apply it creatively in the lab. The effectiveness of the *Virtual CVD* reactor in these very different programs will indicate its true transportability and general usefulness to a variety of academic programs nationwide.

Objective:
        Come up with the "recipe" (i.e. choice process parameters) for a Low Pressure Chemical Vapor Deposition (LPCVD) reactor at as low a cost as possible.

Overview:
        Your team's task is to develop a "recipe" for high volume manufacturing of Silicon Nitride (Si_3N_4) using Low Pressure Chemical Vapor Deposition (LPCVD). The growth and measurements will be made via computer simulation in OSU's *VirtualCVD* reactor. You should develop a recipe that grows Si_3N_4 to a target thickness of 1500 Å uniformly within the wafer and from wafer to wafer. The furnace has a capacity for batches of up to two hundred 300 mm wafers. The wafer spacing is 6.35 mm. It has 5 temperature zones that can be set individually. In addition, you can set the flow rates of ammonia (NH_3) and dichlorosilane (DCS) feed gases, the reactor pressure and the time. You will also have access to a (*Virtual*) ellipsometer, with which you can measure the film thicknesses at the points on any wafer that you select. You will be charged $5,000 for each run and $75 for each measurement (in *Virtual*$, of course)

Deliverables
        Three major deliverables are required: a **design strategy memo**, a **final written report** and a **final presentation** (during the scheduled final exam: 3/17/05 9:30 AM).

A. **Design strategy memo**. You need to come up with a strategy to explore the parameter space. It may be helpful to consider using design of experiments (DOE) in you approach. A tutorial on DOE is available on the class web site. This memo needs to be approved to get your access code to run the *VirtualCVD* reactor. Access codes will only be available the week 2/28 – 3/4.

B. **Final Written Report**. Your report should include the following items:
  i.   Introduction
  ii. Design strategy
  iii. Summary of the results of the runs
  iv. Analysis
  v.   Final recipe
  vi. Final cost

C. **Final Presentation**. Prepare a 10 minute Powerpoint presentation

Figure 8. Sample Student Project Description used in ChE 444/544 in Winter 2005

Table 1. Summary of Student Performance for Winter 2005

Group	Uniformity	Std Error off Target		Cost	DCS Utilization	moles NH3 used
1	99.3%	10.76	$	79,500	15%	3.1
2	99.4%	9.16	$	76,250	14%	2.6
3	99.0%	15.58	$	96,625	23%	1.8
4	98.7%	18.76	$	97,625	1.4%	21.5
5	99.6%	6.40	$	94,050	6%	5.1
6	98.9%	16.03	$	34,975	7%	6.6
7	99.4%	8.31	$	75,125	17%	1.8
8	97.9%	30.96	$	131,250	9%	8.3
AVG	99.0%	14.50	$	85,675	11%	6
STDEV	0.6%	7.92	$	27,304	7%	7
MAX	99.6%	30.96	$	131,250	23%	22
MIN	97.9%	6.40	$	34,975	1%	2

As a demonstration of its versatility the *Virtual CVD* reactor has been adapted to demonstrate Green Engineering (GE) principles through the GE website maintained by Rowan University.[13] In this problem, the student use the *Virtual CVD* reactor to minimize the utilization of dichlorosilane within manufacturing and cost constraints, i.e., the student actually practices Green Engineering. This application shows a strength of the *Virtual CVD* Learning Platform as an educational tool. It can be creatively adapted to fit in and support any number of different curricular structures. It essentially provides a complete system which instructors can use as they need.

Assessment system and evaluation plan
A critical component to the success of this project is the development of an assessment system to evaluate the effectiveness of this tool in promoting higher order thinking skills. The assessment system is based on the evaluation of the educational objectives as well as the transportability of the learning platform.

By using an analytical model based on engineering principles, the reactor outputs are reflective of the chemical and physical phenomena occurring within the system masked by the variation seen in real processes and measurements. Thus those students who integrate their fundamental engineering science knowledge should be more efficient with the experimental designs. We believe this approach will allow conceptual integration of statistics and engineering science and lead to deeper understanding of both topics. In fact, performing the simulation will motivate students to learn more about the physical science to reconcile why they see the results that they are obtaining; thus, they will learn the theory of reactor operation better as well.

The evaluation model that best fits the *Virtual CVD* reactor project is one that closely integrates assessment results to improve the design and implementation of this learning platform in the classroom. Evidence of the development of the cognitive capacity of students requires the design and interpretation of an assessment system that mirrors the ways in which knowledge is developed and applied in the working environment of engineers.[14] Formative and summative assessment tasks will be implemented and evidence about the ways in which the students engage with the learning platform will be made operational. The development of an assessment system tied through backwards design[15] to the educational objectives that frame the content and processes of the courses is viewed to be one of the products of this project. In addition, the evaluation plan will measure the transportability of the *Virtual CVD* Learning Platform to support its use in a variety of engineering and science courses and disciplines.

An initial assessment was performed on the Winter 2005 pilot of the *Virtual CVD* Learning Platform. The assessment data were collected from Likert-scale statements that were part of the overall ChE 444/544 course evaluation. The evaluation statements were designed to assess how well the student felt the course educational objectives were satisfied and to measure the effectiveness of the different learning mediums used in the course. One of the six course educational objectives comes directly from the educational objectives of the *Virtual CVD* Learning Platform listed above. In addition, five learning media were utilized in this course: hands-on labs, traditional homework assignments, industrial seminars, a literature review, and the *Virtual CVD* Learning Platform. These evaluation statements and results are shown in Table 2.

Analyzing these assessment results leads to an interesting juxtaposition. Students felt less proficient with the educational objective concerning the *Virtual CVD,* as compared to the other educational objectives (71% vs. 80%); however, they felt that the *Virtual CVD* was the MOST effective learning medium used in the course --- even more so than hands-on labs (84% vs. 74%). Although the students found the *Virtual CVD* to be effective, after they completed the assignment they only felt moderate mastery of the associated educational objective. These results highlight the complexity of the cognitive processes necessary to perform this task, which is precisely the benefit of early introduction of DOE methodology to engineering students.

The *Virtual CVD* application itself provides useful quantitative data about the student's interaction with the learning platform. A summary of all students' interactions with the tool and all raw data is available. These data are available to the instructor through the instructor interface. An example of this output is shown in Table 1, as discussed above. Another useful assessment tool is analyzing the standard error off target as shown for different axial positions along the reactor as displayed in Figure 9. Interpreting this graph and relating it to the table summarizing student's results, an instructor can assess how well the students optimized the reactor. For example, although Group 4 starts off with only marginal uniformity, their process results in rather consistent monotonically increasing uniformity wafer to wafer, axially up the reactor. Contrarily, Group 3 starts with very good uniformity, however, the axial effects result in very poor uniformity up the reactor. This group has the best dichlorosilane utilization, showing the challenge of increasing utilization while maintaining uniformity. Again, the uniformity monotonically increases along the axis of the reactor. In some cases, the standard error goes through a maximum along the axis of the reactor such as with Groups 2, 6 and 8. In such a case, the students have not optimized the temperature profile along the reactor. In essence, if a group shows a monotonically increasing profile, it has done as good as it can, given the conditions at Wafer 1. The only way they can do better is to change conditions at Wafer 1. On the other hand, groups that show a maximum in this plot have not obtained the optimal axial profile given their

Table 2. Assessment data from Winter 2005 pilot using a Likert-scale
(1=very poor to 6=excellent)

Assessing the degree to which the course educational objectives were met:	Score
I am able to systematically optimize the performance of a CVD reactor for as low a cost as possible.	71%
Combined score for all other objectives	80%
Measuring the effectiveness of learning mediums:	**Score**
The effectiveness of the *Virtual CVD* Reactor assignment was …	84%
The effectiveness of the labs was …	74%
The effectiveness of the homework was …	65%
The effectiveness of the industrial seminars was …	76%
The effectiveness of the literature reviews was …	68%
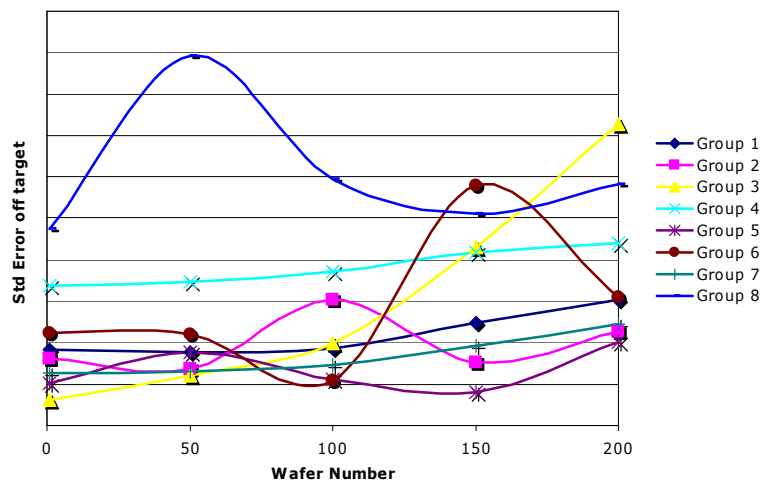
Figure 9. Assessment tool output to instructor - Plot of standard error off target. Shown for the 8 groups using the *Virtual CVD* reactor in Winter 2005.

choice of conditions at Wafer 1. The assessment data available from the summary table and graph of standard error, both available through the Instructor Interface, provide a complete picture of the student's optimization performance.

The assessment data presented above will be included in a more comprehensive plan for Winter 2006 and Fall 2006. Since a central role of the assessment design is development of a model of cognition, experts will be utilized to construct such a model. Previous research has shown the value of observing experts while they "think aloud" to give insight to their cognitive process.[14] This technique will be utilized to construct a cognitive model, and from this an expert-novice comparison will be developed. Additional, qualitative data will be collected through student interviews and focus groups. Another aspect of the assessment plan is designed to illicit evidence of any misconceptions that could interfere with learning, or gaps in knowledge that might inhibit learning. To this end, quantitative data will be collected from a pre-project assessment test. This assessment system will be used in an iterative way to feedback enhancements to the *Virtual CVD*. Information on misconceptions or gaps in knowledge will be incorporated into future revisions of the *Virtual CVD* learning platform. We are implementing the project in several classes over a year period and multiple deliveries provide an opportunity to feedback the results from the assessment to continually improve this high-tech learning tool.

Conclusion
The *Virtual CVD* Learning Platform provides a *capstone* experience in which the students synthesize engineering science and statistics principles. They apply DOE in the context similar to that of industry with a wider design space than is typically seen in the undergraduate lab. The software application contains a 3D graphical user interface, a calculation engine, an instructor interface, and a database. The calculation engine consists of a first principles mathematical model obscured with process and measurement variation. These educational materials will provide a synergy between reinforcing fundamental statistics-based concepts and the engineering science that is emphasized throughout the curriculum. The *Virtual CVD* Learning Platform is self-contained so that it can be placed with versatility where it fits in a given program's curriculum, both within ChE departments and in other appropriate disciplines. It is available for

use upon request. While the platform chosen is specific to the microelectronics industry, it is expected the lessons learned may be applied to any process; hence its delivery at OSU will change from a topic specific elective course to the required capstone lab. Initial assessment results from Winter 2005 show that the students found the *Virtual CVD* reactor to be the most effective learning medium in the course; however, after they completed the assignment they only felt moderate mastery of the associated educational objective. These results highlight the complexity of the cognitive processes necessary to perform this task, which is precisely the benefit of early introduction of DOE methodology to engineering students. Assessment methods are integrated into the instructor interface. A more comprehensive assessment strategy, planned for future offerings, is also described.

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Appendix A: Mathematical model

The overall silicon nitride deposition reaction from dichlorosilane (DCS) and ammonia may be represented by:

$$10\ NH_3\ +\ 3\ SiH_2Cl_2\ =\ Si_3N_4\ +\ 6\ NH_4Cl\ +\ 6\ H_2$$

Assigning molar fluxes towards the wafer surface positive, those of ammonia and DCS are positive while those of ammonium chloride and hydrogen are negative. At the operating temperature for the silicon nitride deposition reaction, there may be dissociation of ammonia to slight extent, which adds negative fluxes of nitrogen and hydrogen as the products of the ammonia dissociation. Hence, the stoichiometry indicates that the sum of fluxes would reduce to a small enough value, and it may be appropriate to assume the equimolar counter diffusion, and the molar flux of ammonia towards the wafer surface may be approximated by

$$N_{NH_3} = J_{NH_3} + x_{NH_3} \sum_i N_i \approx -D \nabla C_{NH_3}$$

where D is the effective diffusivity of ammonia in the gaseous mixture.

The reactor chamber may be modeled as illustrated in Figure A1, being divided into two zones:

(a)   the annular space between the reactor wall and wafer edges, through which gaseous reactants flow and

(b)   the space between adjacent silicon wafers, in which diffusion is the process for the mass transfer of gaseous reactants.

Based on the dimensions of deposition reactors as well as the wafer layout and the deposition reaction characteristics, it may be reasonable to assume for the model development that:

(1)   the system is at pseudo-steady state in terms of the concentration profiles of gaseous components

(2)   the deposition takes place on both the top and bottom wafer surfaces equally,

(3)   the amount of reactants consumed by the deposition of silicon nitride on the liner wall surface is much smaller than that on the silicon wafer surfaces,

(4)   the mass transfer through the annular space is controlled by the convective flow and the contribution of diffusion to the mass transfer in the direction of flow is very small,

(5)   the system pressure is uniform at the operating pressure throughout the reactor,

(6)   the temperature in the space between two adjacent wafers is uniform and equal to the temperature in the annular space next to the two wafers, and

(7)   the deposition rate is of first order with respect to the concentration of NH_3 on the wafer surface.

It should be mentioned that, under the operating conditions adopted for the silicon nitride deposition, the contribution of mass transfer by the Knudsen diffusion is still smaller than that by the ordinary diffusion.

A.1. Mass balance in the space between wafers

Based on the assumptions made above, the mass balance equation of NH_3 in the space formed between the two adjacent wafers and its boundary conditions are:

$$\frac{\partial^2 C}{\partial r^2} + \frac{1}{r}\frac{\partial C}{\partial r} + \frac{\partial^2 C}{\partial z^2} = 0$$

where C is the ammonia concentration though the subscript to represent ammonia has been omitted. The boundary conditions are:

$$C = \text{finite} \qquad \text{at} \qquad r = 0 \qquad \text{for} \qquad -\delta \leq z \leq \delta$$

$$C = C_i \qquad \text{at} \qquad r = \frac{d}{2} \qquad \text{for} \qquad -\delta \leq z \leq \delta$$

$$\frac{\partial C}{\partial z} = 0 \qquad \text{at} \qquad z = 0 \qquad \text{for} \qquad 0 \leq r \leq \frac{d}{2}$$

$$-D\frac{\partial C}{\partial z} = k'C \qquad \text{at} \qquad z = \pm\delta \qquad \text{for} \qquad 0 \leq r \leq \frac{d}{2}$$

where 2δ is the spacing between two adjacent wafers, d is the wafer diameter, and k' is the first-order surface rate constant. The ammonia concentration in the annular space between two wafers at i and $i+1$ is represented by C_i.

The concentration of ammonia at any location in the space between wafer i and wafer $i+1$ is given in terms of its concentration in the annular space, C_i, as a solution of the equations given above, by

$$C = C_i\left(1 - X\right)$$

where the extent of conversion, X, of ammonia in the space between the two wafers is given by

$$X = \sum_{n=1}^{\infty} \frac{2\cosh\left(\lambda_n z\right)\cdot J_0\left(\lambda_n r\right)}{\lambda_n \frac{d}{2} J_1\left(\lambda_n \frac{d}{2}\right)\left[\cosh\left(\lambda_n \delta\right) + \frac{D}{k'}\lambda_n \sinh\left(\lambda_n \delta\right)\right]}$$

where J_0 and J_1 are the Bessel functions of first kind with order zero and one, respectively. The

equation below gives λ_n as multiple root's.

$$J_0\left(\lambda \frac{d}{2}\right) = 0$$

A.2. Local and average deposition rates on wafers

Local deposition rates on the top surface of wafer i and bottom surface of $i+1$ may be evaluated by:

$$\left(\frac{d\lambda}{dt}\right)_{local,i} = \left(\frac{M}{10\rho}\right) k' C_i \left(1 - X_{z=\delta}\right)$$

where $X_{z=\delta}$ may be evaluated by setting $z = \delta$ in X.

The transfer rate of ammonia from the annular space to the space between the two wafers, at i and $i+1$, is given by:

$$F_i = \left| \int_{-\delta}^{\delta} \pi d \left(-D \frac{\partial C}{\partial r} \right)_{r=\frac{d}{2}} dz \right|$$

The average deposition rate on the top surface of wafer i and the bottom surface of wafer $i+1$ is then given by:

$$\left(\frac{d\lambda}{dt}\right)_{average,i} = \left(\frac{M}{5\pi d^2 \rho}\right) F_i$$

and F_i by:

$$F_i = 4\pi d\, D\, C_i \sum_{n=1}^{\infty} \frac{\sinh\left(\lambda_n \delta\right)}{\lambda_n \frac{d}{2} \left[\cosh\left(\lambda_n \delta\right) + \frac{D}{k'} \lambda_n \sinh\left(\lambda_n \delta\right) \right]}$$

A.3. Mass balance in the annular space

The space between the liner and wafer edges may be modeled as a series of well mixed compartments formed by the boundaries located at two adjacent wafers. The concentration in each compartment is assumed to be constant. The model is illustrated in Figure 2. A mass balance about the i-th compartment, bounded between wafers i and $i+1$, is

$$v_{i-1} C_{i-1} - v_i C_i - F_i = 0$$

where v_i is the volumetric flow rate of gas flowing through the annular space.

With the expression for F_i, the mass balance equation may then be rewritten in terms of C_i as:

$$C_i = \frac{v_{i-1}}{v_i + 4\pi d D \sum_{n=1}^{\infty} \frac{sinh(\lambda_n \delta)}{\lambda_n \frac{d}{2}\left[cosh(\lambda_n \delta) + \frac{D}{k'}\lambda_n \, sinh(\lambda_n \delta)\right]}} C_{i-1}$$

where the volumetric flow rate v_i may be given, based on the ideal gas law, with the pressure P and temperature T at the annular location i by:

$$v_i = \frac{F_{total,i} \, R T}{P}$$

The total molar flow rate, $F_{total,i}$, of gaseous reactant leaving location i is given with the stoichiometry of the deposition reaction by:

$$F_{total,i} = F_{total,\,feed} - \frac{1}{10}\sum_{j=1}^{i} F_j$$

where $F_{total,\,feed}$ is the total molar feed rate of ammonia and DCS entering the reactor, and j starts from 1 at the wafer located at the reactant gas entrance.

A.4. Temperature dependencies

Both the surface rate constant, k', and effective diffusivity, D, are dependent on and correlated to temperature T_i at location i as:

$$k' = k'_0 \, e^{-E/RT}$$

$$D = D_0 \left(\frac{T_i}{298}\right)^{1.75} \left(\frac{101300}{P}\right)$$

where k_0' is the pre-exponential factor, E is the apparent activation energy, D_0 is the effective diffusivity of ammonia at 298 K and 101.3 kPa.

A.5. Temperature profiles

The furnace for heating an LPCVD reactor in it is usually divided into several heating zones, and the temperature for each heating zone needs to be determined by an operator. However, the temperature distributions in the reactor are seldom measured and not well characterized. In the model, temperature profiles are hence estimated based on discrete temperature settings at n fixed different locations in the reactor, i.e., T_1, T_2, Λ , T_n, using the constrained cubic spline (Kruger).

Kruger, CJC, "Constraint cubic spline interpolation for chemical engineering applications," http://www.korf.co.uk/spline.pdf.
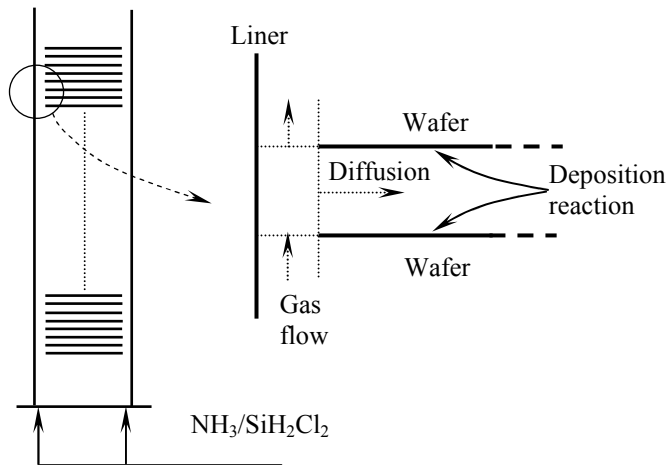
Figure A.1. Modeling of reactor chamber.
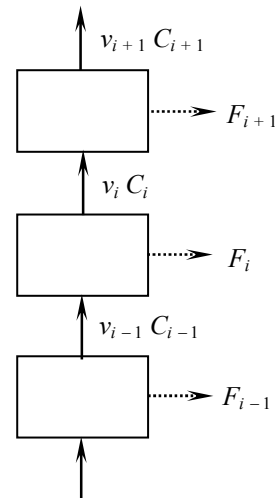
Figure A.2. Modeling annular space.

Appendix B: Software design

The project is designed as a number of independent components. The three main components are the *data server*, the *3D client*, and the *Web interface*. These components are shown in Figure B.1.

At the core of the project is the *data server*. The *data server* acts as the brains of the project: it performs all of the calculations, stores the data, carries out actions requested by users, and sends results back to users. The data server has several sub-components: a *mathematical model* which is used to determine thickness measurements on wafers, a custom disk-based *hierarchical database* used to store user relationships and data measured within each user account, and an *XML-RPC server* which runs as a daemon and handles requests from the outside world.

Including each of the sub-components, the *data server* is 8,000 lines of Python code. The methods exposed by the *XML-RPC server* are rather high-level. For example, a typical student session might involve the following method calls:
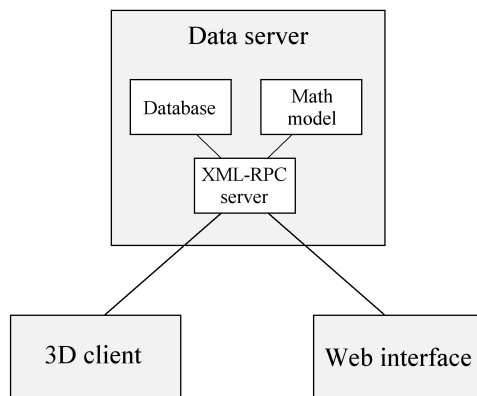
Figure B.1. Main components of VirtualCVD software project.

Description	RPC method
Login and get a session ID.	session_login
Find the number of reactors.	reactor_count
Make a run on reactor 1.	reactor_new_run
Make a measurement set in metrology.	metrology_new_set
View a previous measurement set.	metrology_get_set
Export measurement set as a spreadsheet.	metrology_export_set
Log out.	session_logout

In principle, students and instructors can access the *Virtual CVD* reactor solely through the *XML-RPC server*. In practice, we reasoned that it would be more aesthetically pleasing for end users if measurements were made using a 3D graphical interface, creating a virtual reality fabrication facility. Thus the *3D client* software was created. For instructors, we created a *Web interface*, so that instructors can create student accounts and view the progress of students through a Web browser. It should be emphasized that the latter two components are not strictly necessary for the project; they are front-ends which focus on visual and human aspects, but they do not add to the core functionality exposed by the *data server*.

The *3D client* contains 21,000 lines of C++ code. It consists of several sub-components: the engine, the GUI classes, and the implementation code. The engine is a flexible agent-based system: it contains an abstract base class which all agents inherit from. Here "agent" is a general term that describes any 3D object in the environment. Each agent handles its own visibility testing, rendering, physics, and status update functionality. Thus the core engine is quite simple. The GUI classes implement common widgets such as textboxes, list boxes, and buttons. The actual implementation of the fabrication facility is done by subclassing the engine classes and the widget classes. All graphics are rendered in OpenGL. Animation is done by translating the 3D models. The 3D models were created in the software program Maya by Autodesk, Inc.

The *Web interface* contains 4,400 lines of Python code. It uses a custom Web framework, which consists of a naive search-and-replace templating system, a CGI URL-to-function mapping module, and a cookie-based login system. The built in Python XML-RPC functionality is used to communicate with the *data server*.