

RESEARCH BRIEF

MDPSAS: MODULATED DISTRIBUTED PARAMETER SYSTEM ANALYSIS AND SIMULATION TOOLBOX

The situation

Semiconductor device fabrication is complex, requiring multi-step chemical and physical processes to create silicon-based integrated circuit chips. Typically it includes cleans, photolithography, ion implantation, etching, thermal treatments, chemical (CVD) and physical vapor deposition, molecular beam epitaxy, electroplating, chemical-mechanical polishing, wafer testing and backgrinding.

These processes, some of which take place on the molecular or atom-scale level, are modeled as chemical reaction engineering problems. Along with similarities to traditional chemical process modeling issues are some differences. One of these is a less well-developed understanding of the basic chemical and physical processes at work compared to, say, petro-chemical industries. There also is a more rapidly evolving process equipment and product design time scale.

Simulation-based tools are widely used to supplement experiments and reduce the cost in developing new products and solving manufacturing problems. However, there is a lack of truly flexible simulators that can model the exotic chemical mechanisms at work and account for the large range of time and length scales characteristic of these manufacturing process systems.

The challenge

Semiconductor device feature sizes decrease in each generation, making it important to understand underlying physical and chemical mechanisms in manufacturing processes. Key phenomena often exist at different scales which are governed by different physical laws, and the validity of conventional continuum-based or empirical models applied to these processes becomes questionable. To take into account this multiphysical nature, multiscale modeling methods now are regularly employed in semiconductor processes simulation.

Chemical process design, development and simulation generate large sets of non-linear algebraic

and/or differential equation systems to be solved. There are three general approaches. One is for the *user* to develop the entire simulation program using a high-level programming language. This requires the user to understand the chemical and transport phenomena as well as numerical methods and programming.

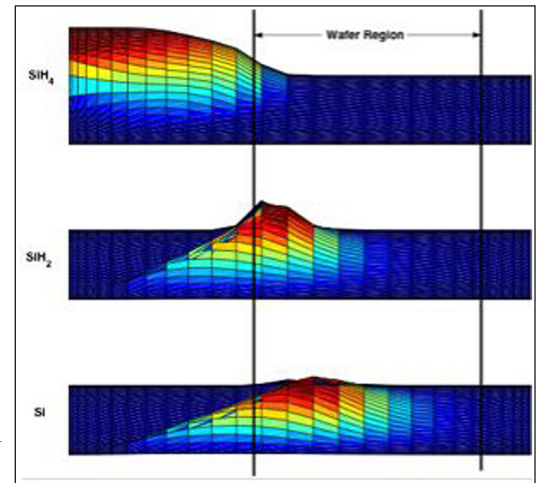
A second approach is to use commercial or other specialized software designed for specific applications.

Or the user may employ a general engineering software

product which develops a full simulation from a combination of built-in modules and user specified elements. A graphic interface helps the user set up problems and run the simulations. Users generally specify the physical domain, transport and chemical processes, and boundary conditions without the need for detailed knowledge of fluid dynamics and computational techniques. Such products include flowsheet tools, used for simulation, design, optimization and control of a complete plant or process; and partial differential equation (PDE) solvers, which simulate distributed parameter systems focusing on detailed transport phenomena within a contiguous spatial region. While powerful, typically the tool is not very flexible or customizable, and also can be expensive.

The research

ISR Associate Professor Ray Adomaitis and his team have developed MDPSAS, a MATLAB-based set of modular simulation tools. MDPSAS is a flexible and



A MDPSAS-generated graph.

extensible structure that can solve a wide range of chemical process simulation problems using object-oriented programming techniques.

Starting with the MATLAB12 general problem solving environment, the team developed a flexible, modular, model building and analysis framework. They incorporated elements of both flowsheet and PDE solvers to allow evolutionary simulator development. A central feature is the inclusion of object-oriented techniques to implement weighted residual methods, which allows the solution of PDE-based models.

The team broke simulation problems into modular components, or subelements, of manufacturing processes. Each module can be solved and analyzed individually, which helps track the source of solution divergence or other numerical problems. Modules can be assembled by combining elements and defining how information is exchanged between modules. This makes it possible to define modular systems combining lumped and distributed parameter models, which then become a reusable part of the modeling library.

Modular modeling is effective in describing equipment hardware elements as well as reaction mechanisms and simulator elements that do not necessarily correspond to physical equipment components. The ability to solve and test individual modules along with the ease with which modules can be combined, solved, analyzed, and swapped in and out simplifies simulator construction and debugging, and facilitates evaluating model elements. The framework facilitates an “evolutionary” approach to simulator development, starting with a simple process description and building model complexity and testing hypotheses in a step-by-step manner.

Design patterns offer a high-level abstract structure to avoid dealing with programming details early on. This makes designing more efficient and fosters a better understanding of object-oriented analysis and design. The framework currently is implemented using MATLAB, but proposed design patterns will allow users to create modular systems with object-oriented programming languages of their choice.

The simulation framework is capable of determining numerical solutions to model modules described by non-linear algebraic equations, ordinary and partial differential equations, as well as any combination. Boundary-value problems are

(semi)discretized with a built-in quadrature-based MWR procedure, and the framework interfaces to the full suite of MATLAB ODE/AE solvers.

Research team

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Software download

Current version of mdpsas: www.isr.umd.edu/Labs/CACSE/A-Team/mdpsas/mdpsas.zip.

Demo of the CVD thermal model: www.isr.umd.edu/Labs/CACSE/A-Team/mdpsas/CVDthermal.zip.

For more information

Dr. Adomaitis's home page: www.isr.umd.edu/faculty/gateways/adomaitis.btm.

Dr. Adomaitis's research group: www.isr.umd.edu/Labs/CACSE/A-Team/.

J. Chen and R. A. Adomaitis, “An Object-Oriented Framework for Modular Chemical Process Simulation with Semiconductor Processing Applications.” *Computers and Chemical Engineering*, 30, 1354–1380 (2006).

The software was featured at a seminar on Capitol Hill organized by the American Association for the Advancement of Science: www.aaas.org/news/releases/2007/0625insurgents.shtml.