Global Headquarters: 5 Speen Street Framingham, MA 01701 USA P.508.872.8200 F.508.935.4015 www.idc.com

WHITE PAPER

Modeling and Simulation: The Return on Investment in Materials Science

Sponsored by: Accelrys Inc.

Michael Swenson Michael Languell, Ph.D.
James Golden, Ph.D.
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IDC OPINION

Based on in-depth interviews with materials research scientists and engineers, IDC concludes that there is a significant return on investment (ROI) to be realized from the use of modeling and simulation software tools in partnership with traditional experimentation. The use of modeling and simulation software, or in-silico research, is gaining in use in materials science just as it has in other fields such as pharmaceutical R&D. Our models, derived from conversations with researchers at major companies, suggest a cumulative ROI on the order of $3 to $9 for every $1 invested in these tools and associated expertise. The degrees of benefit vary considerably by the type of user (occasional, power, or specialist) but are consistent in the type of benefits realized. The highest levels of ROI are achieved through the use of internal modeling and simulation specialists and a well-integrated team approach that emphasizes coordinated, iterative work with experimentalists.

In addition to revealing the intellectually satisfying benefit of a deeper understanding of the underlying physics and chemistry of materials, this white paper has uncovered the following types of benefits that are amenable to quantification:

- Experimental efficiency
- Broader exploration of materials solution space
- Product development "saves"
- Modeling and simulation testing of safety margins and avoidance of expense and liability related to hazardous materials
- Improved time to market for new products

METHODOLOGY

The objective of this white paper is to examine and develop estimates of the return on investment (ROI) for using modeling and simulation computational tools/software in the area of materials science.

The primary source of information for this white paper comes from a series of in-depth interviews conducted by IDC analysts with users of modeling and simulation tools from a variety of companies engaged in materials science and engineering. Eleven interviews were conducted: eight in person, one via written correspondence, and two via teleconference. The interview notes were written up and then circulated back to the interviewees to ensure accurate representation of their examples and viewpoints.

From those stories and examples, we developed ROI scenarios with specific estimates of factors. These estimates circulated back to interviewees, giving them an opportunity to examine and react to the scenarios and associated estimates. Additional feedback at this stage from interviewees contributed to significant clarification of assumptions and estimates.

Throughout this study, IDC deliberately chose what we believe to be conservative estimates for assumptions used to build the ROI scenarios. Some of the case studies show more dramatic returns, but each individual company must take into account its own situation and market when estimating existing or potential ROI.

Please see the Appendix for specific examples of how estimates were derived from interviews.

IN THIS WHITE PAPER

This white paper discusses the range of typical costs for deploying modeling and simulation tools and the supporting computational infrastructure. The paper then goes on to delineate and discuss four distinct, yet related, benefit scenarios. An example ROI is calculated for each scenario. Case studies are interwoven throughout to help illustrate the various scenarios.

SITUATION OVERVIEW

Return on investment (ROI) is an underlying concern for all forms of business. This paper focuses on the ROI that can be realized in the development of innovative materials through the use and application of modeling and simulation software. Specific case studies are employed to demonstrate how savings can be realized through gains in experimental efficiency, broader experimental evaluation, rescue of stalled product development projects, and risk management by safety testing. The investment methodology for materials (IMM) described by Maine and Ashby (*Materials & Design*, 23 [2002], 297–306) provides the perfect framework for this discussion.

Investment Methodology Overview

High risk and long lead times between invention and a marketable product characterize innovations in the materials industries. These two aspects of materials development carry with them very high costs. The IMM proposed by Maine and Ashby can sharply reduce these costs. IMM consists of three interconnected parts: viability assessment, market forecasting, and value capture.

Material Viability

The viability of a new material for a particular application is dependent on the balance between its technical and economic attributes. The technical attributes of a material run the gamut of properties (e.g., physical, mechanical, thermal). The properties, known or theoretical, of the new material can then be compared to the profiles of existing materials. This modeling of the properties for a material tells but half the story. The other half of the equation is made up of the economic attributes. The economic attributes are cost and value and can be harder to establish. The costs of a new material include primary production and secondary processing. Because the material is new, we generally do not have the benefit of historical data to calculate the production costs. The only recourse is to use materials processing simulation to properly capture these costs.

Market Forecasting

Although the market value of a new material is an estimated parameter, when the performance metrics are coupled to the inputs of customer requirements and emerging opportunities, then such information as target markets and material development focus can be obtained. This analysis results in two options: (1) identification of new markets or applications or (2) substitution into an existing market. Should a material be deemed viable and a suitable market for its introduction discovered, then the final hurdle for the product is value capture.

Value Capture

Having a viable material and a suitable market for its sale is insufficient in and of itself. Investors must be convinced that they will be able to capture the value and obtain an economic ROI. A discussion of the role that modeling and simulation can play in this arena follows.

Modeling and Simulation

In materials science and engineering, modeling and simulation are used in a variety of contexts, including:

Modeling of Materials Properties

- Mechanical (ultimate strength, toughness, hardness)
- Thermal (heat capacity, thermal expansion, thermal conductivity)
- Electrical (conductivity [and resistivity], dielectric behavior)
- Chemical (reactivity, corrosion rates)
- Optical (refractive index, spectral absorption)
- Magnetic
- Nuclear (radioactivity, half-life, neutron absorption cross-section)

Simulation of Materials at Different Length Scales

- Electron (quantum mechanics)
- Atomistic (molecular mechanics and dynamics)
- Mesoscale processes (mesoscale modeling)

Accelrys, the sponsor of this study, offers application suites targeted at these functional areas, including the following products:

- Materials Studio
- Cerius2
- Insight II

ROI Models and Case Studies

Developing a Cost Model

In the typical materials science R&D environment, we have observed the following ranges of costs associated with deploying these types of modeling and simulation applications (see Table 1):

TABLE 1

Modeling and Simulation Cost Model

Item	Annual Cost	Notes
Software licenses	$35,000 to $100,000	Range depends on specific applications and modules.
Computational resource (low end)	$5,000	Desktop PC or laptop and access to a Quad processor Pentium Xeon server.
Computational resource (medium)	$50,000	Unix workstation — small Unix server or small Linux cluster.
Computational resource (high end)	$100,000	Unix workstation — plus access to a medium-sized Unix server or larger Linux cluster.
Training	$5,000	Higher first year — lower in subsequent years — assumes one or two events per year that include workshops.
Internal IT support	$1,000 to $10,000	Depends on the scale and complexity of the server environment used.
Labor	$0 to $150,000	At the low end, there is no incremental labor cost because these tools are simply being added to the portfolio of tools available to an experimental scientist/engineer. At the high end of the price range, the ROI model assumes that a company hires a person to work as an internal consultant applying modeling and simulation to a wide variety of projects.
Total	Ranges from $46,000 on the low end to about $370,000 on the high end	Low-end costs are for adding this set of modeling and simulation software to the complement of tools for an experimentalist. High-end costs include tools and computational support plus the salary and benefits of a specialist.

Source: IDC, 2004

For the purpose of calculating the ROI for various benefit scenarios discussed below, we have characterized three "typical" users of modeling and simulation tools. First, there is the experimentalist who is an occasional user of modeling and simulation tools. This class of user has his or her cost set toward the low end at $50,000 per year (see Table 2). That price assumes the low end of licensing and of computational support. It is assumed throughout the document that this type of user applies modeling and simulation tools and techniques to four projects per year.

The second type of user defined is the experimentalist who is a power user of modeling and simulation tools. His or her annual costs are set at $80,000 with a more robust set of applications and computational support. We assume a power user will apply modeling and simulation to about eight projects a year.

The final type of user is the modeling and simulation specialist (often a computational chemist by training). The annual cost for the specialist is set at $350,000 based on the high end of the range of application licenses and computational support and the addition of salary (see Table 2). The two types of experimentalist users do not have salary added into the cost model because, presumably, they would be hired as experimentalists without regard to modeling skills. We assume, due to greater efficiency at computational projects and the nature of an internal consultant role, that a specialist will apply modeling to about 18 projects per year.

Having defined the cost side of the equation, we now move to examining multiple benefit scenarios.

Scenario 1: Efficient Experimentation

If we recognize that an experimentalist can quickly test a theoretical material through modeling and simulation, then we can deduce reductions to direct experimental costs.

Assumptions and Logic for Annual Benefits

- The average cost of an experiment ranges from about $500 to $30,000. A rough midpoint of $13,000 is chosen for the ROI calculation in this model.
- Each project is assumed to consist of 10 experiments on average.
- Estimated efficiency savings are 15% for the occasional user, 20% for the power user, and 35% for the specialist. We note that some of our case study examples indicate higher levels of savings, but we err on the side of conservative estimates to assure the reader that the projected returns are achievable.

Table 2 shows that the ROI based on experimental efficiency ranges from $1.56 to $2.34 for the occasional user and the specialist, respectively. This means that for every dollar invested in using modeling and simulation, the R&D department should realize at least $1.56 in savings.

TABLE 2

Scenario 1: Experimental Efficiency

Type of Employee	Annual Number of Projects	Average Experimental Cost of Project	Percentage of Savings	Total Annual Benefit	Cost	ROI
Experimentalist and occasional user of M&S	4	$130,000	15%	$78,000	$50,000	$1.56
Experimentalist and power user of M&S	6	$130,000	20%	$156,000	$80,000	$1.95
M&S specialist	18	$130,000	35%	$819,000	$350,000	$2.34

Source: IDC, 2004

We understand that the role of the specialist is not fully accounted for in this model, since the specialist could, or should, also have broader and more comprehensive knowledge of a variety of tools. The specialist can contribute to some projects that the experimentalist cannot. Furthermore, having one or a few specialists in the company increases the value of experimentalists in that company doing modeling: the specialists can develop and recommend computational protocols that the experimentalists can use. The specialists also steer the experimentalists away from problematic approaches and toward useful ones. Specialists tend to also have a better skill set and knowledge base for interpreting the results and know the pitfalls of the employed techniques.

In support of the above assumptions in improved efficiencies, we offer the following case studies taken from investigators working on actual problems and projects. The first is provided by Mike Makowski, Ph.D., at PPG.

> Mike Makowski, Ph.D., is a principal investigator (PI) and head of modeling for the R&D group at PPG, a diversified manufacturer of protective and decorative coatings; sealants; adhesives; glass products; and industrial, specialty, and fine chemicals. Dr. Makowski shared a number of insights on the use of modeling and simulation in the R&D labs of PPG. First, he emphasized that although modelers are still occasionally called upon to help rescue a project, they are more commonly involved with new R&D projects from the start. When modelers are involved from the start of a project, the modeling and simulation work is seen as a guide to experimental work.
>
> The improvements in productivity can be quite substantial. Dr. Makowski reflected on a recent product development team for a new industrial powder-coating market. This cross-disciplinary team included marketing people to help define the desired end

properties, synthesis chemists to develop the desired properties, and formulation chemists to work on manufacturing processes and formulations. Modelers were included to help throughout the process. This project, including the patent submission, took 3 to 6 months. Similar efforts without modeling and simulation support typically take 9 to 12 months. The modeling and simulation for this project were such that Accelrys software running on a P4 laptop could handle the task, though some runs took as long as 5 hours. In the worst case, effective use of modeling and simulation was estimated to cut product development time in half, saving potentially hundreds of thousands of dollars in development expense, in addition to enabling the recognition of revenue from a new product months earlier.

A second example provided by Dr. Makowski is in the development of organic light emitting diodes (OLED). In this case, the challenge is to simultaneously optimize for color, quantum efficiency, and overall brightness of the device as well as power efficiency of the overall device. Each cycle of deciding on, synthesizing, and purifying a candidate molecule as well as making and then testing a device for appropriate properties can take anywhere from 6 to 12 months. The modelers used historical data on dyes for color properties and predictive models developed for some of the other properties to devise an overall modeling run that would predict whether molecules would have the desired properties, thus avoiding the 6- to 12-month cycle until they were fairly confident that a candidate molecule was likely to succeed. Using modeling software and 4 processors on an SGI Origin 3000, each candidate molecule took about 24 hours to run. Each candidate that was conclusively shown not to work through in-silico means can be seen as avoiding 3 to 6 months of experimental work. In addition to direct savings in avoided experimental costs, this approach raises the probability of finding an optimal end product because it was economical to search through and "test" a much broader set of potential molecules for the OLED products.

A second case study is provided by Dr. Ryuzo Tanaka, Central Research Laboratories, Idemitsu Kosan Co. Ltd.

Dr. Ryuzo Tanaka has been charged with investigating and increasing the use of computational chemistry tools and techniques in the central R&D function of Idemitsu Kosan Co. Ltd., a Japanese oil company. In the past, these tools have been used occasionally in scattered instances, but the company is developing a centralized expertise that can serve researchers in multiple business units.

Dr. Tanaka emphasizes that the company is being realistic about the adoption of computational chemistry tools such as molecular dynamics. While the company certainly expects to realize significant benefit from these tools, it sees them as another set of tools to use along with traditional experimental techniques. Benefits that the company expects to realize from tools such as Discover, DMOL3, CASTEP, and QSAR in Accelrys' Materials Studio include:

- Lower costs through more focused experimentation
- Improved knowledge management
- Improved ability to predict and design properties for lubrication products, electric materials, and refining catalysts under development
- Improved time to market

Dr. Tanaka also acknowledges that not every research chemist is ready to accept computational chemistry tools. This is partly a generational issue that will improve over time, but it is also important to carefully position these tools as one among many and not overpromise on the capability of modeling and simulation tools.

Scenario 2a: Broader Exploration

As a result of improved experimental efficiencies, the experimentalist can engage in broader explorations of improved materials and compounds. Table 3 summarizes the assumptions and calculations for uncovering the ROI related to product improvements that flow from broader exploration of solutions enabled by the use of modeling and simulation tools.

TABLE 3

Scenario 2a: Broader Exploration

Type of Employee	Annual Number of Projects	Percentage of Projects Generating a Product Improvement	Value of 1% Share of Market	Total Annual Benefit	Cost	ROI
Experimentalist and occasional user of M&S	4	7%	$1,000,000	$42,000	$50,000	$0.84
Experimentalist and power user of M&S	6	12%	$1,000,000	$108,000	$80,000	$1.35
M&S specialist	18	20%	$1,000,000	$540,000	$350,000	$1.54

Source: IDC, 2004

For the purpose of analyzing this scenario, we have utilized the following benefits estimates:

- Assume a relatively small market of $100 million in total annual sales for a product category including all competitors.
- A fairly conservative estimate is that a noticeably better product may yield a market share improvement of 1% that will last for 2 years before competitors are able to respond and gain back their lost share.
- The incremental share growth in this scenario would be worth $2 million over the 2-year period or $1,000,000 annually.

Not all of the incremental market share value can be attributed to modeling and simulation, even though it may have provided the critical insight that made the improvement possible. Investments are also made in new materials, possibly in new tooling, and in marketing the improved product. We estimate in Table 3 that modeling and simulation efforts account for 15% of the responsibility for the improved product and market share. The "Total Annual Benefit" column is calculated as follows: number of projects x percentage of projects generating an improvement x value of 1% market share x 15%.

However, we note the conservative sizing of the product category market. In most product markets, a 1% share is worth considerably more than $1 million per year. Similar impact on larger markets would raise the ROI calculations considerably. Companies participating in much larger product categories can easily justify the investments in modeling and simulation.

The following case study serves to highlight some of the benefits gained from broader exploration through the application of computational modeling and simulation in materials research.

> In our discussion with the head of scientific computing for a global manufacturer of chemical products, we learned that modeling and simulation on many different levels have become deeply ingrained in the R&D process. Each major line of business within the company supports its own experimental chemists, but the modeling and simulation group is part of the central R&D function and thus its members serve as internal consultants on research projects sponsored by each line of business.
>
> The group's structure brings together experts from a variety of modeling disciplines ranging from finite element modeling to molecular modeling. In this organization, modeling and simulation have been recognized by the central R&D leadership as vital to the organization. To overcome resistance to using modeling within some of the line-of-business R&D groups, the central R&D organization funds the modeling group so that its services can be offered "free" to the line of business. This lowers any access barriers for research managers who remain skeptical of the value.

> The manager who heads up the modeling and simulation group indicates that while it is difficult to track the individual financial impact of the group on the diverse projects to which it contributes, he does ask the line-of-business vice president to write a letter of recommendation at the close of each project that articulates the group's contributions. This internal documentation of value has increased the usage of the modeling and simulation group throughout the R&D functions. Examples of the value delivered include:

- Reduction in time to market
- Reduced experimental cost per project
- Better understanding of the scientific underpinnings of experimental outcomes
- Improved manufacturing processes
- Acting as a catalyst for sharing knowledge and best practices across the various R&D units

> Another indicator of the value that these modeling and simulation experts deliver to the organization is that they are now routinely invited into the beginning of new R&D projects rather than being seen as a rescue squad for troubled projects. In this way, the work of the modelers becomes more iterative and integrated with that of the experimentalists.

Scenario 2b: Deeper Understanding

The greater use of modeling and simulation will lead to an improved understanding of the fundamentals of the pertinent phenomena. This improved understanding may be captured in a database, which will contribute to the development of material informatics. This body of information can then be used by less experienced researchers to make advancements normally reserved for more senior personnel.

A quantitative ROI for this scenario is difficult to calculate, but based on the experiences shared below, the value added is undeniable.

Dr. Shigeru Yao, manager of the Materials Design department and leader of the Nanotechnology Promotion group for the Polymer Research Laboratory of Corporate Research & Development for UBE Industries Ltd., offers the following:

> The R&D department of UBE Industries Ltd. designs new "specialty chemicals" that deliver high value through inclusion in pharmaceutical products or creating materials with specific functional properties. The manipulation of materials to create functional properties is an important goal of the emerging area of nanotechnology. This technology that controls material structures on the atomistic or molecular level enables the development of unique innovative functions as well as incremental improvements to

existing materials and processes. Computational chemistry is exploited by UBE Industries Ltd. as a dominant approach to creating novel nanomaterials.

In looking back almost 15 years, Dr. Shigeru Yao, who doubles as manager of the Materials Design department and leader of the Nanotechnology Promotion group in the Polymer Research Laboratory of UBE Industries, reflects on the circumstances leading to adoption of computational chemistry. "Around 1990, while there was a trend toward new polymeric material development, it appeared that the property-estimation method based on empirical rules had reached the limit. At that point, we adopted software that deals with molecular mechanics and molecular dynamics; that was our starting point in using computational chemistry."

Currently, UBE Industries uses several molecular simulation solutions from Accelrys, such as "Materials Studio," a material molecular design platform; "Discover," which calculates molecular mechanics and molecular dynamics; and "MesoDyn," which calculates coarse-grained dynamics, from design of polymer materials to design of catalysts.

Dr. Yao continues, "It is now a common occurrence in our organization to hear questions about the results from a simulation. It appears that computational chemistry techniques are becoming more widely appreciated, and routinely used, as the number of our scientists and engineers using Accelrys' solutions increases."

It is said that the value of the adoption of molecular simulation is due to the reduction of time and cost by rationalization of the R&D process. Dr. Yao explains, "You cannot tell whether or not target function and property are actually obtained until the material is finally made. But it costs time and money to do so. If it becomes clear that the targeted function does not emerge during simulation, you can stop it in the early stages. And it is very important that the reason can be rationally explained, not as simply the feeling that '"It may fail.'"

He continues, "If the R&D process depends on only conventional experiments or intuitions of the researchers, it is difficult to conclude "No go" on a proposal. It is also not easy to conclude "Go" and persuade the company to proceed.

"Especially for young researchers, simulation is good training for acquiring theoretical thinking. It leads to an understanding of the fundamentals of the phenomena and provides young researchers a basis for asserting their idea to veteran researchers. If experience and knowledge are captured and preserved in a database, it should at some point become possible for even inexperienced researchers to explore and investigate the potential in new materials."

> By computerizing "experiences" and utilizing them systematically, researchers contribute toward the development of materials informatics and eventually the creation of a research field called "materials design," according to Dr. Yao.

Scenario 3: Saving a Product Development Project

Two case studies provide examples of how modeling and simulation were used to rescue product development projects that were at a standstill and on the verge of being cancelled. In one case, it was relatively early — after about 10 months of experimentation and the involvement of several researchers, the effort to develop a new compound was about to be abandoned. With only three days of modeling and simulation by an internal specialist, a new compound was designed that met all the design parameters and is now headed to market. In the other case, a new glass fiber had been developed, but an unusual defect was discovered during accelerated life-cycle testing. Isolating the cause of the defect would have taken months of additional work via experimentation, but modeling and simulation solved the problem in a matter of weeks. The manufacturing process was changed to exclude the defects, and the product was brought to market successfully.

The benefits in these situations clearly depend significantly on the size of the relevant markets for the products. The assumption for this scenario is that a new product will yield $1 million a month in new incremental revenues if it is successfully brought to market. We also assume that a company has already spent $6 million in R&D on this product. If the use of modeling and simulation saves the product from being cancelled and allows it to proceed to market, what might that be worth?

- **Option 1.** Cancel the product — never make it to market — $6 million in development plus 3 years of lost revenue at $12 million per year = $42 million.

- **Option 2.** Delay the product launch — assume it takes 6 months of additional work and another $500,000 in development costs to solve the problem through conventional means. Benefit is $500,000 in avoided development costs and 6 months of revenue at $6 million = $6.5 million.

Most researchers, using modeling and simulation, rarely have a "save" of this obvious magnitude. In a larger company with many product development projects under way simultaneously at any given time, an experienced specialist may enable a save like this once every 5 years. What is not clear is how many "save" situations are avoided because researchers used modeling and simulation along the way in an iterative fashion with experiments, instead of waiting for a project to reach a crisis point.

Table 4 outlines the estimates and calculations for a product development save. We see that the expected annual ROI ranges from $1.04 for the occasional user to $4.18 for the specialist.

TABLE 4

Scenario 3: Product Development Save

Type of Employee	Annual Number of Projects	Percentage of Projects Generating a Save	Value of a Save	Total Annual Benefit	Cost	ROI
Experimentalist and occasional user of M&S	4	0.20%	$6,500,000	$52,000	$50,000	$1.04
Experimentalist and power user of M&S	6	0.75%	$6,500,000	$292,500	$80,000	$3.66
M&S specialist	18	1.25%	$6,500,000	$1,462,500	$350,000	$4.18

Source: IDC, 2004

What follows are three accounts that elucidate the mechanism of saving a product development project. These examples show clearly the role that computational modeling can serve in materials research and development while supporting the assumptions made in the ROI calculations.

Brian Peterson, Ph.D., Computational Materials Science, Computational Modeling Center, Air Products and Chemicals Inc.

> Brian Peterson, Ph.D., has 15 years of experience as a molecular modeler. He has spent the past eight years in the Computational Modeling Center at Air Products and Chemicals Inc. in Allentown, Pennsylvania. The Computational Modeling Center combines scientists and engineers with a variety of specialties, including computational fluid dynamics, molecular modeling, statistical modeling and analytics, and advanced optimization analytics. This multidisciplinary modeling team serves as an internal consulting team to other more traditional R&D teams. When asked how his group demonstrates the value of modeling and simulation in its materials research setting, he talked about the necessity of keeping an internal account of the success or failure of each project.
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> One example of the value that his group provides is when it was asked to assist with a project that was having trouble with the separation process for a product for the electronics industry. Through the course of analyzing the process using modeling tools such as Cerius2 and Materials Studio, the modeling group concluded that one of the failed experiments should have actually succeeded. Upon re-running the experiment, the group confirmed the modeling; the earlier failure was due to troubles with the execution of the experimental procedure. This analysis helped the

company ship the product on time and within specification when it appeared that neither criterion would be met.

However, Dr. Peterson also indicated that much of the value his group creates is more subtle and harder to track. In many cases, the modeling group is more integrated into the flow of the R&D work and makes contributions along the way, including guiding experimentation in more fruitful directions. One critical type of decision the group often helps make are "stage-gate" decisions. These go/no-go decisions are very familiar to the pharmaceutical industry in the evaluation of targets and leads, and in materials science and engineering, there are similar stage decisions where work on a new compound must be evaluated and resources either allocated for further development or reallocated to another compound or another project altogether. Modeling and simulation analysis often helps by indicating the relative probability of success among several compounds under development. The ability to fail potential compounds early through analysis of the underlying physics has important financial benefits for the corporation, but current accounting systems and practices are not designed to record and track money saved from failing early.

Dr. Peterson acknowledges that not all R&D managers are willing to accept modeling and simulation as a valuable tool. However, as some managers repeatedly use the modeling group with good effect on their projects, the success stories circulate through the larger organization and help to overcome the resistance of some managers.

One important element for helping to integrate modeling into the larger R&D environment is to provide some central funding so that modelers can answer the one-off, short questions for line-of-business researchers without having to ask for a budget number to apply it toward. This lowers the barrier for getting the modelers involved and often allows them to solve the problem in the time it might otherwise take to just get approval to solve the problem.

Senior Research Associate, Major Glass Products Manufacturer

This researcher has a long history of combining experimental science with modeling and simulation in the investigation of areas of glass research ranging from photosensitive properties, to durability issues for glass polymer composites, to interaction of surfactants with ceramic batch materials. In the everyday workflow, he seamlessly moves back and forth between experiment and calculation. Modeling and simulation are primarily used to help him look in the right direction and to clarify the theoretical underpinnings for the work he is doing. For example, an experiment may yield a material with a desired property. He will then use modeling and simulation software to help uncover the molecular or atomic basis for the observed property. Once the underlying mechanism is understood, he can create a family of materials with the same property and begin to optimize that property along with other desired properties in the final material.

While it is difficult to account directly for the increase in productivity that this blending of modeling and simulation with experiment provides, his company has clearly come to believe in its value. It supports this capability through licensing Accelrys software such as Cerius2 and Materials Studio. It further supports him by providing a dedicated SGI workstation as well as access to shared computational resources in a central datacenter.

Occasionally this researcher gets involved in "firefighting," solving critical problems for a product. One story he tells is of the work on an optical fiber product. During testing, the fiber was subjected to a variety of conditions, including high heat. The testers observed that the fiber showed unusual optical attenuation after the heat test. An examination of the literature and the company's own data showed that this attenuation due to heat had no precedent. A hypothesis was made regarding defects during the consolidation phase of manufacturing the fiber; however, the company had no way to empirically locate and measure the defect. This researcher then used molecular modeling techniques to simulate the chemistry of the manufacturing process. The modeling demonstrated that a particular type of molecular defect, if exposed to oxygen during consolidation, would result in a fiber with the observed attenuation problems. The company changed certain manufacturing processes, the problem was solved, and the optical fiber went to market.

Although modeling and simulation were only one small part of the total effort to bring this fiber to market, they were critical to solving a gate-type step in getting to market. Until this problem was solved, the fiber was not going to market. Such dramatic interventions on applied products can have a very large ROI for a company that has invested in both the tools and the expertise to deploy modeling and simulation in the materials science area. If this problem had not been solved by any other means, the product might never have come to market, and the company would have forgone millions in revenue. It is possible that the problem would eventually have been solved through continued experimentation and testing. However, even under this scenario, the modeling and simulation work probably displaced several months of additional experiment and testing. As a result, the company avoided potentially hundreds of thousands of dollars of expense while improving short-term revenue by preventing months of delay in getting to market.

Michael York, Research Scientist, Continental Tire Division, Materials Development

> Continental Tire had initiated a project that was scheduled to take one year to develop and test a new compound with improved properties for a new tire product. Initially the project did not include modeling and simulation. After nine months of experimentation, the project appeared to have made no noticeable improvements over the compound used in prior products. At that point, Research Scientist Michael York was asked to use his experience in forensic chemistry and his expertise in modeling and simulation tools to help the project get back on track.
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> Using tools such as Discover, DMOL3, RMMC, Amorphous Cell, Polymer Builder, and Conformer, the company undertook a modeling and simulation exercise. The data from the nine months of experimentation was used to help set parameters of known "failures." The properties of the existing production compound were used as the benchmark for measuring improvement.
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> After three days of modeling and simulation, Continental Tire had a new compound to synthesize and test. The modeling and simulation indicated that the new compound would have the desired improvements in properties over the existing compound and provided insight into the reasons for the failures of the previous nine months of experiments.
>
> The dramatic difference in time to solution and, ultimately, the ability to design new compounds that result in improved tires have convinced Continental Tire of the ROI for modeling and simulation software applications and the computer hardware to support those applications. While no one expects modeling and simulation to take over from bench chemistry and experimentation, Continental Tire has recognized that modeling and simulation are a key component of successful materials science and engineering. It is increasing its commitment to the use of modeling and simulation by training additional chemists in the use of these tools and equipping them with the necessary applications.

Scenario 4: Risk Management Through Safety Testing

There are materials that are designed to perform vital functions in extreme environments. Aerospace applications, for instance, face extremes of temperature, gravitational forces, vibration, and mechanical stress loads as well as high levels of radiation. While some of these extremes can be successfully replicated in physical test environments, others are neither easily nor economically replicated. Modeling and simulation can play a key role in predicting how materials will react under these extreme conditions or combinations of the extreme real-world conditions. Failures under extreme conditions can have very dramatic human and economic costs for aerospace programs. All too well known are the deaths of astronauts, delays in space programs, reassignment of personnel to conduct disaster analysis, and loss of confidence from funding agencies that are part of the multimillion dollar consequences of dramatic failures. Any weaknesses identified through modeling and simulation that would have otherwise gone undetected can be invaluable.

Although most products do not face these kinds of extreme conditions, many other products can benefit from additional detailed analysis to mitigate risk. One aspect of safety testing is the area of hazardous materials. Consider the case in which experimentalists are considering using a new compound for an application. This new compound may be hazardous to either manufacture or use. The costs associated with a hazardous material (or process) are twofold. First, prior to any experimentation, an extensive hazard review process has to be completed. Typical costs for this review alone are around $10,000. Then, should the compound (or its manufacturing process) prove to be hazardous, specialized equipment will have to be built. Specialized equipment by its very nature is expensive and can push the price of the project well beyond the high-end estimation of $300,000 (10 experiments per project x $30,000 per experiment) used in the first ROI scenario.

Modeling at this point can serve two functions. A demonstration through modeling that the new compound will not meet the requirements for the application results in a "No go" on the material or possibly on the project itself. Although this is essentially the same as the first ROI scenario (experimental efficiency), the cost savings are considerably larger. One of these projects alone would nearly pay for the services (software and equipment) of a specialist for a year. A second possibility is that if one can prove beforehand that there is a significant safety hazard, be it that the experiment is too hazardous or that the product is unsafe for the market, again very high cost savings are realized.

Although the variability from situation to situation is extraordinarily high in this scenario, we offer a sample set of estimates and calculations in Table 5. With the value of avoiding a hazard or liability set at a relatively low $2 million per discovery/incident, and the rate of a researcher making such a discovery estimated as very rare (1% to 3% of projects), we still estimate an ROI of $1.60 to $3.09 per dollar invested for the occasional user and the specialist, respectively. The actual value of a liability avoidance could easily be one or two orders of magnitude higher, which in turn would cause a much higher ROI estimate.

TABLE 5

Scenario 4: Safety Testing and Hazard Avoidance

Type of Employee	Annual Number of Projects	Percentage of Projects with a Hazard or Safety Element	Value of Hazard or Liability Avoidance	Total Annual Benefit	Cost	ROI
Experimentalist and occasional user of M&S	4	1.0%	$2,000,000	$80,000	$50,000	$1.60
Experimentalist and power user of M&S	6	2.0%	$2,000,000	$240,000	$80,000	$3.00
M&S specialist	18	3.0%	$2,000,000	$1,080,000	$350,000	$3.09

Source: IDC, 2004

The following comments from a materials engineer again describe the possible benefits in this area and simultaneously point out the obstacles that must be overcome to fully implement this technology.

> A materials engineer from a major aerospace company shared the following insights on the use of modeling and simulation software for R&D projects within his company. This engineer, a long-term user of molecular modeling and simulation tools, argues that molecular modeling is currently where finite element modeling was 30 years ago. Namely, that it can now solve real problems but is still not universally accepted by chemists and materials engineers. Despite resistance from some "old-school skeptics," he finds many project leaders ready to deploy his skills as a modeler on their projects. The benefits realized by his R&D peers include the following:

- Improved failure analysis and understanding of safety margins in conditions that are hard to duplicate in the lab but that might be experienced in extreme cases
- Elucidating the scientific basis for measured variability in material properties
- Providing a quantitative estimate of properties that are currently "immeasurable" — particularly important in very leading-edge technology development
- Working with bench chemists to quantify and validate their intuition before money is spent on synthesis and testing
- Reduced development time through working closely with experimentalists

> As an example of ROI, this engineer cites projects that may last for up to a year and have a budget of roughly a million dollars for experimentation. With each experiment running to several thousand dollars, spending a few hours to do in-silico screening is easy to justify. The in-silico screening might eliminate a number of working hypotheses as either running into a physical impossibility or having a very low probability of working. By focusing the experimentalists' attention on the remaining plausible hypotheses, the modeling specialist aids in reallocation of both material and human resources and improves the probability of a successful outcome for the project.

The following comments from Dr. Scott Owens, Cchem. MRSC, senior research technologist at Nuclear Sciences and Technology Services, British Nuclear Fuels (BNFL), plc, reinforce the safety benefits as well.

> Dr. Scott Owens, senior research technologist for British Nuclear Fuels, plc, shared his experiences in integrating chemical modeling into the broader research and development environment within BNFL. Traditionally, chemical modelers had been a separate group that focused on atomistic quantum and molecular mechanics. However, recently they have been integrated into a larger modeling group that includes experts in computational fluid dynamics, process modeling, finite element modeling, and environmental modeling.
>
> For one major responsibility of the organization — maintaining the safety and operability of the British reprocessing and power plants — all types of modeling are critical because experiments are often expensive and can result in wastes that require treatment or disposal. More broadly under the BNFL umbrella, modelers provide assistance to a number of distinct research and development tasks ranging from disposal of nuclear waste to process improvements and waste stream cleanup. Dr. Owens suggests a number of guiding principles from his own experiences:

- Communication with engineers is critical in order to understand the underlying materials questions more thoroughly
- Integrate chemical models into engineering models to fully communicate the findings and drive home the practical benefits
- Reassure engineers that your work is complementary to theirs
- Focus on the ability to "de-convolute" complex interactions
- Deliver value around safety models — in-silico versions of experiments that cannot be conducted
- Develop information that guides rather than replaces experimentation
- Successful projects are enabled by close collaboration between experimentalists and modelers

As a specific example of the ROI for modeling, Dr. Owens pointed to a task in which the chemical modelers were asked to assist in modeling a vitrification process for waste disposal. Because of the intense heat and corrosiveness of the melt, the containers used for the vitrification process last only a few weeks. Each flask costs about £90,000 (US$160,000 at current exchange rates). Their modeling efforts helped to understand why the melt containers were failing and thus suggested changes to the design of the container to extend its useful life without requiring significant plant modification. In addition to the extended usable life of an expensive component, the long-term benefit in having to dispose of fewer containers and achieving increased throughput through less downtime is even larger, providing a long-term ROI of potentially millions of pounds.

Total ROI

If we employ computational modeling and simulation in materials research, what is the anticipated magnitude of ROI for the above scenarios? Table 6 summarizes the findings.

TABLE 6

ROI Summary

	Scenario 1: Experimental Efficiency	Scenario 2a: Broader Exploration	Scenario 3: Product Development Save	Scenario 4: Safety Testing and Hazard Avoidance
Experimentalist and occasional user of M&S	$1.56	$0.84	$1.04	$1.60
Experimentalist and power user of M&S	$1.95	$1.35	$3.66	$3.00
M&S specialist	$2.34	$1.54	$4.18	$3.09

Source: IDC, 2004

While it is tempting to simply sum these ROI calculations, we recognize that there is some overlap. For example, the savings from experimental efficiency can be reinvested into broader exploration. In our opinion, the benefits from Scenarios 3 and 4 are significantly more independent. Thus, if we estimate that all of the savings in Scenario 1 are reinvested in the remaining scenarios but are otherwise additive, we conclude with a combined ROI of about $3 for every dollar invested in tools and support for the occasional user, about $8 for every dollar invested in tools and support for the power user, and just under $9 for every dollar invested in both salary and tools for the specialist. These returns will be a function not only of the employee skill set, business area, and maturity of computational structure but also of the corporate culture. Strong sponsorship by executive management is critical to obtaining a healthy ROI (both tangible and intangible) in computational modeling and simulation in materials.

It is important for readers to understand that these calculations are examples using a certain set of reasonable, even conservative, assumptions. Any particular business considering the adoption of modeling and simulation tools for materials research should conduct a careful analysis of the similarities and dissimilarities between these estimates and 'its own situation. Some of the case studies indicated an ROI that would be considerably stronger than the estimates used in the various scenarios. However, readers should recognize that these cases represent organizations and people with years of experience in applying modeling and simulation to materials research. First- or second-year returns might not be as robust.

CHALLENGES/OPPORTUNITIES

Challenges

Unfortunately, any tool or technology can deliver substantial benefits to an organization only if it is utilized correctly and effectively. As mentioned in several of the case studies, there exist real but surmountable challenges to the implementation of computational modeling and simulation in materials research. Some of those challenges are:

- Initial investments in software, computing resources, and access to expertise can result in a fairly significant up-front cost, particularly for smaller companies.
- A fairly steep learning curve exists for the tools themselves and for the proper interpretation of the results.
- Not every experimentalist has the mathematical skill and theoretical background to use these tools effectively.
- Molecular modeling can solve real problems, but it is not yet universally accepted by chemists and materials engineers. This skepticism can hinder full integration into the workflow and cause a less-than-optimal ROI.
- Current accounting practices are not designed to record and track money saved from failing early.

The presence of these challenges and barriers means that it is important for modeling and simulation to enjoy the support of R&D management. Some of our examples show that it is ideal if the modeling and simulation function is supported financially from a central fund so that individual R&D project managers will feel comfortable bringing in internal specialists to help on a project.

Time-to-Market Opportunity

Although not always explicit in the case study interviews or in the scenarios developed from those conversations, one important way in which strong ROI can be realized is in an aggressive application of modeling and simulation tools to the challenge of reducing time to market. In Scenario 2a, we discussed how improvements in experimental efficiency often lead to broader explorations of potential solutions and occasionally directly contribute to a product improvement and ultimately market share. Certainly, broader explorations can be curtailed once a "good enough" solution is found and the remaining efficiencies are translated into faster product development cycles.

While time-to-market improvements are an implicit option in Scenario 2a, they are an explicit component of the product development save in Scenario 3. IDC believes that businesses engaged in markets where time to market is highly critical and materials engineering issues are significant can deliberately invest in and direct the use of modeling and simulation tools as a development accelerator.

CONCLUSION

In summary, we can safely say that real and significant cost savings and financial benefits can be garnered from the use of computational modeling and simulation in materials research and development. The mechanisms for these gains are:

- Increased experimental efficiency leading to the reduction of direct research costs
- Efficiency gains leading to broader and deeper exploration of solutions and new products
- Financial gains by improving the time to market for new products
- Revenue gains from the rescue of stalled product development projects
- Risk management through safety testing and failure analysis

Real, but non-quantitative, benefits can also be realized. As an example, what value can we place on an improved understanding of the fundamentals of the phenomena that control experimental outcomes? This is particularly important in the training of younger researchers. Not only will researchers' morale be strongly influenced in a positive direction if they experience more successful projects in the lab by avoiding untenable solution paths, but companies will benefit from better work from a more productive staff operating in a more collaborative environment.

APPENDIX

Methodology Examples

The following are specific examples of how we arrived at estimates contained in the ROI scenarios.

In "Scenario 1: Experimental Efficiency" (refer back to Table 2), we needed to estimate what percentage of experiments are typically avoided through the use of modeling and simulation. In this case, we started with one of our most dramatic case study interviews, which indicated that a 24-hour modeling and simulation run replaced 3 to 6 months of experimental work. Further, the implication was that many of these modeling runs were completed before deciding which compounds to actually begin experimenting on. While none of the other interviewees had as dramatic an example of efficiency gains, they almost universally indicated that guiding experiments in more fruitful directions, thereby increasing experimental efficiency, was a key element of how they deliver value to their organization. From these observations, we formulated specific, more conservative estimates for the scenario (savings of 35%, 20%, and 15% for specialists, power users, and occasional users, respectively). And, as stated in the Methodology section, these scenarios were circulated by the interviewees for an assessment of reasonableness.

Another example of how we arrived at estimates is in "Scenario 2a: Broader Exploration" (refer back to Table 3). We estimated that 15% of the product improvement that was initiated by an insight arrived at through modeling and simulation should be attributed to the modeling and simulation. There is no direct way to allocate this, so the estimate is based on the following logic. A product improvement in this case flows directly from an insight generated by modeling and simulation and thus the percentage granted should not be trivially small. On the other hand, it should not be overstated either, since many other departments and functions within a company are needed to bring that product improvement to market. After discussion, we settled on a figure of 15% as a compromise between "trivial" and "overstating" the impact. Ultimately, what we have created is a model of ROI. Readers should ask themselves what value their own organizations would place on the initial insights that eventually create a product improvement and substitute that percentage for our estimate of 15%.

A third example of how we arrived at estimates is in "Scenario 3: Product Development Save" (refer back to Table 4). We needed estimates of how frequently a researcher would be able to use modeling and simulation to rescue a stalled product development project. In talking with our interviewees, we specifically probed those who described a product development save to estimate how often something like this occurs. One specialist was able to point to a couple of dramatic cases in about a 10-year span. Another power user indicated that he had one dramatic example and didn't expect more than a couple of these in his career. From those kinds of comments, we calculated percentages that would match those levels of frequency: 0.2%, 0.75%, and 1.25% of projects for occasional users, power users, and specialists, respectively. Again, these estimates are drawn from actual cases, but readers are free to substitute their estimates based on their own experience or other data points.