Materials Modelling: expectations, benefits and Key Performance Indicators (KPIs)

Main type of outcome expected

There are basically two different ways in which modelling is applied, either seeking specific data or looking to discover new insights and understanding[i].

A. Data:
   1. Certain, specific property data with a pre-defined/expected accuracy; low number of data
   2. Property data for screening purposes, large amount of data
B. Discovery: gain insights and understanding
   1. Specific phenomena
   2. Broad field
   3. Visual exploration

Benefits and Key Performance Indicators

The following is a collection of benefits and Key Performance Indicators that have been identified in a number of studies[ii,iii] and direct interactions with industrial end users.

1. Improved, deeper insight and understanding, hence:
   a. Avoid dead-ends in R&D
   b. Ability to link materials chemistry/structure to application performance
   c. Enables better informed decisions about material, product and processing choices
   d. Avoid upscaling issues and lower risk of market introduction; reduction of product failures during manufacturing, and after manufacturing
   e. Support trouble-shooting of material/product failures
2. R&D strategy development, e.g. via early exploration of behaviour in downstream applications
3. Broader exploration
4. Fail early, innovate faster
5. Solve problems which could otherwise not be solved
6. More efficient and targeted experimentation, saving time and cost of experiments
7. Avoiding potentially hazardous experimentation
8. Lower cost to obtain certain property data (e.g. due to cost of experiment or synthesis)
9. Estimate property data for materials that cannot be obtained for competitive reasons.
10. Support broader IP claims.
11. Support defensive IP publishing, i.e. pre-empt competition patents.
12. Avoid destructive testing.

13. Faster optimisation of material, formulation and/or process
14. Design innovation and quicker identification of materials.
15. Solutions to design problems.
16. Faster and less costly new product development.
17. Better control of the manufacturing process.
18. Improved capabilities for predicting engineering system performance or life cycle.
19. Virtual engineering assessment of new materials that might be considered risky to assess with physical prototypes.
20. Virtual engineering assessment in systems where the validation of materials performance by system-level testing is expensive, time consuming, or not possible.
21. Faster time-to-market for new products.
22. Market advantage based on improved performance from incorporating materials and processes optimized for particular applications and on more precise modelling of a material's response to an application environment.
23. Improve value chain interactions
    a. Validation of supplier information
    b. Build customer trust
    c. Demonstrate competitive advantage via competitor materials based on models
24. New types of business: from Product to Product +, i.e. Product plus relevant "Model" (typically the relevant Materials Relations) to enable customer to build engineering models faster)
25. Support digitalisation
26. Communication and marketing via models and their visualisation

Quantitative indicators

The following metrics have been used in various studies[iii,iv]

Simple quantitative indicators

1. Number of Models in use in the R&D organisation
    a. For Physics Based models: number of validated/tested Materials Relations
2. Cost saving
3. Number of innovations (product, process, business) achieved
4. Jobs created

Return on investment

Simplest measure that has been applied is: Revenue generated from a project involving modelling / investment in materials modelling for the project (people, software, hardware)

A more detailed calculation is shown below, based on the study by IDC[ii] and reproduced here from Ref [iv].

Cost

The cost C is calculated as:

C = SW + HW + IT + L + T,

Where:

SW = Software,

HW = Hardware,

IT = IT support,

L = Labour,

T = Training.

Benefit

Benefits are evaluated based on a certain qualitative KPI such as

- More efficient experimentation.
- Broader exploration and deeper understanding.
- Saving a product development project and/or accelerated product development.
- Risk management through safety testing.

For each scenario the benefit is estimated by a formula of the form:

$B = Vt \times Np\ (C) \times R(C)$

Where:

B=Benefit attributed to modelling.

Vt = total commercial value of the respective mechanism.

Np (C) = Number of projects that involve modelling, which is a function of the resource available, hence cost.

R (C) = Percentage of modelling projects that make an impact on the mechanism, which is also found to depend on resource, with highly skilled/trained staff with good equipment more likely to make an impact.

The table below includes the data for low end, occasional user and the high end specialist cases as in the IDC study carried out in 2003/4. In addition, a third column provides an updated scenario for a typical modelling user today with a lower cost base due to the reduced price of hardware as well as software since the original study. On the other hand, it was also assumed that the user will not be as highly skilled as some of the experts that were interviewed by IDC, hence the number of projects impacted was reduced from 18 to 10. Nevertheless, the return on investment is substantial.

1	**Efficient Experimentation**	**Low**	**High**	**Updated**
	Cost per experiment	13000	13000	13000
	Experiments per project	10	10	10
	Number of projects impacted	4	18	10
	Reduction on experimentation	15%	35%	50%
	Benefit	**78,000**	**819,000**	**650,000**
	ROI	**1.56**	**2.34**	**2.81**

2	**Innovation due to broader exploration**	**Low**	**High**	**Updated**
	Total market size for product category	100,000,000	100,000,000	100,000,000
	Market share increase resulting from project	1%	1%	1%
	Percentage of Projects Generating a Product Improvement	7%	20%	20%
	Number of projects impacted	4	18	10
	Contribution from modelling	15%	15%	15%
	Benefit	**42,000**	**540,000**	**300,000**
	ROI	**0.84**	**1.54**	**1.30**

3	**Saving stalled projects**	**Low**	**High**	**Updated**
	Percentage of projects saved	0.20%	1.25%	1%
	Value of save, Development cost per project	6,500,000	6,500,000	6,500,000
	Number of projects impacted	4	18	10
	Benefit	**52,000**	**1,462,500**	**812,500**
	ROI	**1.04**	**4.18**	**3.52**

4	**Risk Management Through Safety Testing**	**Low**	**High**	**Updated**
	Percentage of Projects with a Hazard or Safety Element	1%	3%	3%
	Value of Hazard or Liability Avoidance	2,000,000	2,000,000	2,000,000
	Number of projects impacted	4	18	10
	Benefit	**80,000**	**1,080,000**	**600,000**
	ROI	**1.60**	**3.09**	**2.60**

DIRECT BENEFITS	**Low**	**High**	**Updated**
More efficient experimentation	78,000	819,000	650,000
Broader exploration	42,000	540,000	300,000
Saving stalled projects	52,000	1,462,500	812,500
Risk management	80,000	1,080,000	600,000
Potential TOTAL DIRECT BENEFITS	**252,000**	**3,901,500**	**2,362,500**

DIRECT COSTS	**Low**	**High**	**Updated**
Software licenses	35,000	90,000	40000
Hardware	6,000	100,000	30000
Training	7,000	2,000	3000
IT support	2,000	8,000	8000
Labour	0	150,000	150000
TOTAL DIRECT COSTS	**50,000**	**350,000**	**231,000**
ROI estimate	**3**	**9**	**7**

R&D productivity

According to Paul et al[v] R&D productivity P can be expressed as:

$$P \;\alpha\; [WIP \times p(\mathrm{TS}) / (CT \times C)] \times V \quad = [\text{Volume of Innovation/Cost}] \; x \; \text{Value}$$
$$= \quad \text{R\&D Efficiency} \quad x \quad \text{R\&D effectiveness}$$

Proportional to:

- the work in process (WIP): the amount of research being conducted simultaneously
- the probability of technical success (p(TS))
- the value (V)

Inversely proportional to

- cycle time (CT)
- cost (C).

Note however, that most of the above elements are inextricably linked to one another.

The above equation expresses overall R&D productivity as a product of efficiency (volume of innovation divided by cost) and effectiveness (i.e. value).

Using this approach, Paul et al were able to analyse R&D productivity in the pharma industry.

References

[i] E. J. Maginn, "From discovery to data: What must happen for molecular simulation to become a mainstream chemical engineering tool," AIChE Journal, vol. 55, no. 6, pp. 1304-1310, Jun. 2009.
[ii] M. Swenson, M. Languell, and J. Golden, "Modeling and Simulation: The Return on Investment in Materials Science," Jun. 2004.
[iii] G. Goldbeck and C. Court, The economic impact of materials modelling (2016), https://doi.org/10.5281/zenodo.44780
[iv] G. Goldbeck, The economic impact of molecular modelling, (2012), https://doi.org/10.5281/zenodo.44359
[v] Paul, Steven M., Daniel S. Mytelka, Christopher T. Dunwiddie, Charles C. Persinger, Bernard H. Munos, Stacy R. Lindborg, and Aaron L. Schacht. "How to Improve R&D Productivity: The Pharmaceutical Industry's Grand Challenge." Nature Reviews Drug Discovery, November 19, 2010. doi:10.1038/nrd3078