



Materials Modelling: benefits and Key Performance Indicators (KPIs)

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Benefits and Key Performance Indicators

Qualitative

1. More efficient and targeted experimentation, saving time and cost of experiments
2. Deeper understanding
 - a. To avoid upscaling issues and lower risk of market introduction
 - b. To make better informed decisions about material, product and processing choices
 - c. To support trouble-shooting
 - d. Avoid dead-ends
3. R&D strategy development, e.g. via early exploration of behaviour in downstream applications
4. Broader exploration
5. Avoiding potentially hazardous experimentation
6. Lower cost to obtain certain property data (e.g. due to cost of experiment or synthesis)
7. Estimate property data for materials that cannot be obtained for competitive reasons.
8. Support broader IP claims.
9. Support defensive IP publishing, i.e. pre-empt competition patents.
10. Avoid destructive testing.
11. Faster optimisation of material, formulation and/or process
12. Design innovation and quicker identification of materials.
13. Solutions to design problems.
14. Faster and less costly new product development.
15. Better control of the manufacturing process.
16. Improved capabilities for predicting engineering system performance or life cycle.
17. Virtual engineering assessment of new materials that might be considered risky to assess with physical prototypes.
18. Virtual engineering assessment in systems where the validation of materials performance by system-level testing is expensive, time consuming, or not possible.
19. Faster time-to-market for new products.
20. 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.
21. Improve value chain interactions
 - a. Validation of supplier information
 - b. Build customer trust



- c. Demonstrate competitive advantage via competitor materials based on models
- 22. 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)
- 23. Support digitalisation
- 24. Communication and marketing via models and their visualisation

Quantitative

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 (costs for people, software, hardware)