Strategies for industry to engage in materials modelling

HOW TO INTEGRATE MATERIALS MODELLING INTO R&D FOR MAXIMUM BUSINESS IMPACT?

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Executive Summary

The objective of this White Paper is to support industry on the road to making materials modelling and simulation an integral part of research, product development, upscaling and product life cycle management, thereby contributing to enhanced innovation and competitiveness of European industry on a global level.

Representatives of a range of materials and manufacturing companies contributed to the strategy development in expert meetings and surveys to clearly articulate end-user needs. They identified what barriers need to be overcome to introduce materials modelling into their business cycle or enable an enhanced and more efficient/higher quality use of it and what future developments they foresee to be necessary. They also provided their input regarding a range of tools adapted by the EMMC to probe the state of the industry and provide a framework for strategy development in companies.

A key objective was to assess the impact of materials modelling on an organisation and several useful frameworks, tools and metrics are discussed. First of all, Enterprise Business Levels awareness support analysing and aligning materials modelling activities and strategies with business processes at different levels, from specific tasks to macro processes such as the overall R&D process.

Considering further the role of modelling in R&D processes, an augmented Quantitative Benchmark for Time to Market framework is introduced, which we termed the 4D-QBTM. The QBTM provides a means of analysing and tracking the impact of materials modelling on different stages of R&D while the 4D stands for the four dimensions that provide ‘levers’ for impact: People, Tools, Process and Data. The importance of appropriate KPIs is also highlighted. These can be classified in KPIs that track efficiency (such as speed of getting data) as well as effectiveness such as the probability of advancing to the next stage using materials modelling. Also, KPIs can be distinguished for different levels of business processes within an organisation.

Assessing the economic impact of materials modelling on industrial prosperity requires inclusion of benefits and raising awareness, that gaining benefits often requires to do things differently. Benefit management is introduced as vehicle to assure benefits are materialising.

Several industry representatives contributed their assessments to a materials modelling maturity study from which the current materials modelling state of the art could be established. The current state is promising and so is the awareness of barriers that impede the wider adoption of materials modelling in industry. These representants were also able to give ideas how to overcome these barriers and contributed vividly to suggesting change strategies.

Finally, some strategies are outlined to aid materials modelling and simulation becoming an integral part of product life cycle management and making a strong contribution to enhance innovation and competitiveness on a global level.

1. Background

The Roadmap of the European Materials Modelling Council (EMMC, 2018) portrays a vision of European manufacturing industry that has employed materials modelling as an operational practice to develop sustainable and competitive products. The integration of materials modelling and informatics is considered future critical for more agile and sustainable product development and use throughout the entire materials life cycle. It is aligned with the drive towards digitalisation that assists in developing a circular economy and addresses societal needs. A much wider and deeper integration of materials modelling is a goal that is both feasible and necessary. It is feasible since the technology has matured and become much more widely applicable due to a combination of scientific, algorithmic, data science (e.g. Machine Learning), software and hardware developments. It is necessary since more efficient, tailored and agile product development and manufacturing processes as well as new digital operation and business models depend on interconnected model based approaches that include everything from the product to its materials and chemistry (BOEING, 2015).

In the US, the Materials Genome Initiative (MGI), a strategic effort spanning multiple federal agencies, is promoting a globally competitive U.S. manufacturing sector by addressing important gaps in the materials innovation infrastructure. A recent report based on extensive industry interviews (Scott, Walsh, Anderson, O'Connor, & Tassey, 2018) points out that materials modelling, machine learning, data, interoperability, etc, play a dominant role in technology infrastructure needs for advanced materials innovation.

NASA commissioned a roadmap for integrated, multiscale modelling and simulation of materials and systems (Liu, Furrer, Kosters, & Holmes, 2018) and their vision for 2040 is "*A cyber-physical-social ecosystem that impacts the supply chain to accelerate model-based concurrent design, development, and deployment of materials and systems throughout the product lifecycle for affordable, producible aerospace applications.*" Similar efforts are also documented by the U.S. Department of Defence who look into a digital engineering strategy for their equipment. (DoD, 2018)

These roadmaps and reports have in common that they can evidence why industry needs materials modelling in order to stay innovative and develop new materials faster. The reports revealed that several stakeholders from academia, government and industry have to work together to make this happen and reap the benefits. MGI (Scott, Walsh, Anderson, O'Connor, & Tassey, 2018) estimated the potential economic benefit of an improved materials innovation infrastructure of between $123 and $270 bn per year, which is beneficial for both the manufacturer and the consumers (Goldbeck & Court, 2016).

However, improving the use and integration of materials modelling in a manufacturing company requires a strategy based on a careful analysis of current status, benefits sought, identification of changes required and enablers that help bring about the change. This White Paper will provide a framework for the understanding and analysis of relevant business processes, how they can be enhanced by materials modelling and what factors (or dimensions) need to be considered to determine changes that can be employed for organisations to reap the benefits that materials modelling can bring.

2. Big picture – Strategy and Business Process

2.1. Setting the scene

In today's world an industrial organisation will aim to define a business process, which comprises a set of activities leading to a desired outcome, and their logical order and dependence (Aguilar-Saven, 2004). This business process can be analysed and can undergo "modelling" to improve an organisation. Business processes describe generally a series of steps performed by a particular group of stakeholders to achieve a concrete outcome and these processes vary from organisation to organisation. Hence, if we want to engage industry in materials modelling, we have to find out what these processes are to assure modelling can become an asset to an existing process by improving it. While in detail these processes are as individual and as numerous as there are organisations, we can identify typical processes and stages describing R&D as we focus on the discovery, development, manufacturing and deployment of products involving new or enhanced materials.

In order to enable an analysis that connects materials modelling to the business level, we will work with six generic process levels (Viljoen, 2013) that reflect particular stakeholder activities and a hierarchy ranging from individual tasks to enterprise processes (Figure 1).

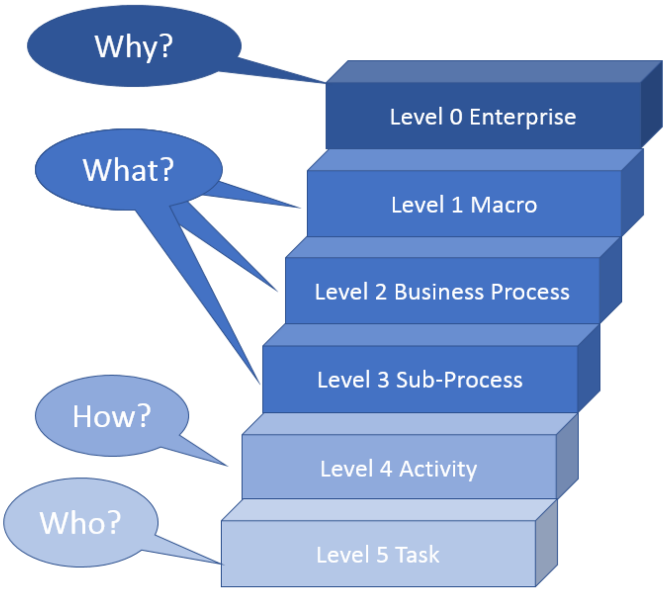

Figure 1: Six levels of a generic business processes: Level 0 answers why something is done, levels 1-3 provide increasing granularity of what needs doing, level 4 deals with how something is done and level 5 comprises who is doing it.

Level 0 – Enterprise is the top level and reflects the business model of the organisation. It is informed by organisational competence, resources, global trends and opportunities. These factors and in particular market analysis lead to requirements for products and new materials to make an impact. Performance at the Enterprise level will be measured with KPIs such as growth, market share, profitability and share price.

Level 1 – Macro Process or Value Chain represents the internal activities an organisation engages in as it transforms ideas into actual products. Value chains will also undergo analysis as one has to establish what each process will cost, how long it takes, what is the chance of success and failure and how to save costs. Also, a value chain can aid to establish which stakeholders in an organisation are needed to maintain and support it. Organisations will also use these value chains to see how they can bring value to their customers. A framework for the materials development value chain has been developed by the US Materials Genome Initiative; Quantitative Benchmark for Time to Market framework, QBTM, (Nexight Group, 2016) identifies four stages: Design, Development, Manufacturing and Deployment (Figure 2). Key Performance Indicators at this Macro Process level are the cost, duration and probability of success for each stage, as will be discussed in more detail in Section 2.2.1

Modelling provides an important lever on the KPIs of the Value Chain, for example it can increase efficiency and reduce the risk of late stage failure as issues can be detected prior to lengthy experimentation.

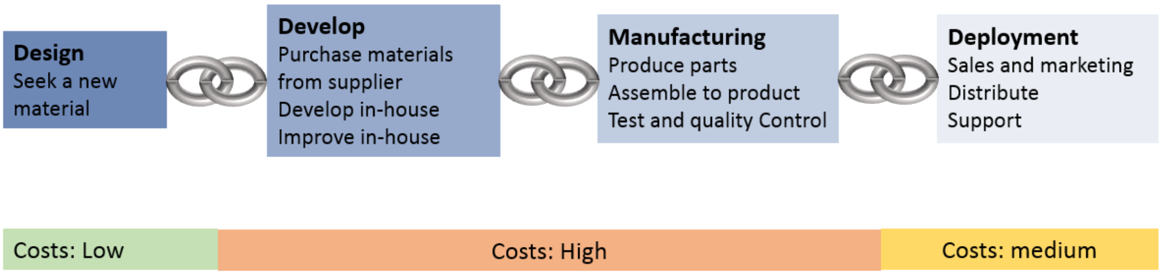

Figure 2: Value Chain with generic cost expectation

Level 2 – Business Process: Each chain link of the macroprocess can be detailed further as a Business Process. For example, the “Design” stage is considered in more detail (Figure 3) and a workflow is described that states what is needed to get a new material which subsequently can be fed into the “Develop” stage. Key to the success of a business process is to take into account the requirements of other processes along the value chain, the macro-environment and the sub-process capabilities. The materials modelling based Business Decision Support System, BDSS (Belouettar, et al., 2018) play a key role here, as they are designed to combine materials models with other sources of information, turning it to actionable knowledge that drives business decisions based on selected KPIs. The latter would for example include measuring the success of this design stage. Impacts of materials modelling on a business process and their measures (e.g. ROI) have been discussed in detail in a previous report (Goldbeck & Court, 2016).

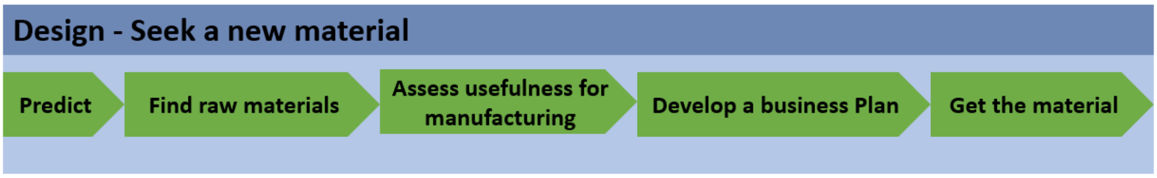

Figure 3: Breakdown of the Macro Process “Design” into Business Processes

Level 3 - Sub-Process: Each business process can again be split in individual processes (Figure 4). In this particular example, one sets up processes that are needed to predict new materials such as literature and databases searches, to make sure the wheel is not reinvented. Then, there will be experimental and *in-silico* screening to find unknown materials. ROI or NPV can be used as quantitative approaches to capture the value of materials modelling within a sub-process.

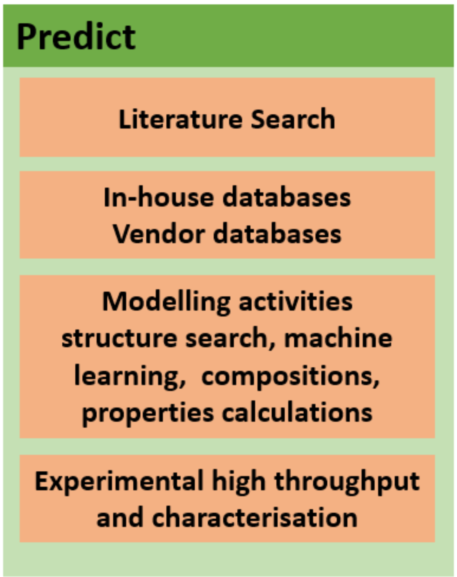

Figure 4: The business process "Predict" is split into Sub-Processes

Level 4 – Activity: A group of individuals will be assigned to actively work on a sub-process. Project management tools will be put in place and Gantt Charts, Kanban boards or similar will put a time line to each activity. A metric for determining whether to perform specific activities should be performed is net present value (NPV). However, care must be taken to keep the big picture, i.e. higher-level processes in mind. For an illustration of the pitfalls of using NPV in R&D decision making (and the advantage of using a question-based approach), see the Introduction Chapter of the thesis (de Viesser, 2003).

Level 5 – Task: The above activity can be broken down into a series of Tasks, for example a simulation. A good way to record a modelling workflow would be a MODA (CWA 17284, 2018) (EMMC, 2019), including a flowchart (Figure 5). Such high-level workflow analysis of Tasks provides and efficient way of discussing and capturing different approaches and supports the important role of translating requirements stemming from high levels to the Task level.

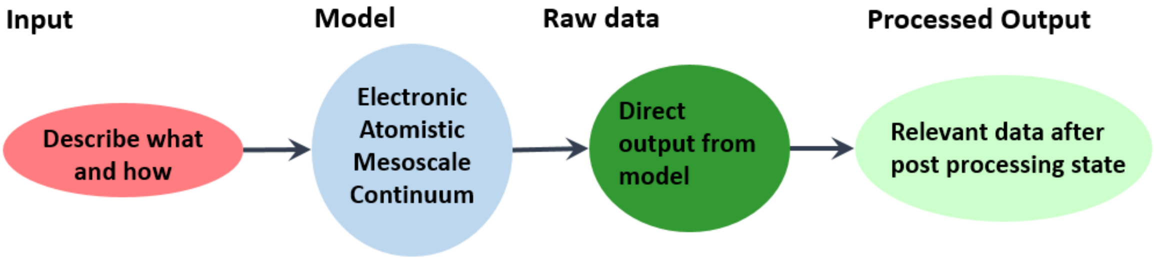

Figure 5: Schematics of a MODA flowchart

2.2. Impact assessment of Materials Modelling in Industry

Materials Modelling needs impact assessment if one wants to justify why it should be part of a business process. In the following sections, we will discuss methodologies mentioned above as they have been applied to materials modelling, i.e. the Quantitative Benchmark for Time to Market framework (QBTM), Return on Investment (ROI) and Net Present Value (NPV). All of these may be required to support an assessment across different business levels. QBTM applies to the Macro and Business Process Levels, ROI is mostly used for Business Processes, Sub-Processes and Activities and NPV for the Sub-process, Activities and Tasks (Figure 6).

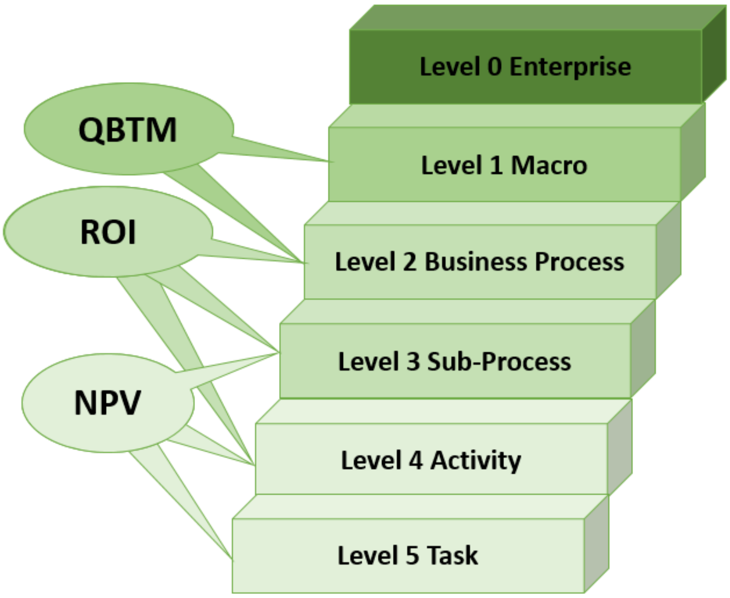

Figure 6: Types of impact assessment linked to relevant business process levels

2.2.1. Quantitative Benchmark for Time to Market framework (QBTM)

This four-stage R&D process model as a basis for benchmarking time to market was established by the US Materials Genome Initiative (Nexight Group, 2016). The resulting framework (Table 1) provides individual organizations with approaches and tools for self-assessment against relevant industry benchmarks. It is beneficial to use a generic framework as time to market for materials innovation varies significantly by material type, function/application, and industry. QBTM is a four-stage framework applicable to a range of materials innovations, the four stages being discovery, development, manufacturing and deployment. Each stage has three phases, Start, Process, and End and to each phase a time duration should be assigned. The framework can be used to analyse previous projects ("reverse roadmap") and indicate where modelling contributed to discrete events (e.g. milestones), and acted (or could have acted) as a factor that decreased the time needed to complete an activity (or "accelerators"). It can also unveil factors that increased the time needed to complete an activity (or "inhibitors"), and it can be discussed whether modelling could help to reduce those.

Table 1: Generic analytical framework for time to market for materials innovation. Four stages are introduced: Design, Development, Manufacturing and Deployment. Adaption of Nexight Group, 2016, Fig 6.

	Stage 1 Design	**Stage 2 Development**	**Stage 3 Manufacturing**	**Stage 4 Deployment**
START	Demand for a new material	Synthesis of materials, lab scale	Synthesis on industrial scale	A commercial product
PROCESS	Experiments and Materials Modelling on lab scale	Scale up to pilot scale Characterisation	Production trials Modifications evaluation	Can be modified, tailored, supported
END	Candidate materials are identified	Materials are identified for industrial scale up with promising properties	Production happens and standards/specifications are established	The product is sold and used

Organisations can use this template (Table 1) and adapt it to their specific workflows and known time durations. For example, the QBTM model was retrospectively applied to materials developments at Corning (NIST, Gorilla Glass, 2016) and QUESTEK (NIST, QUESTEK, 2016). Corning's "Gorilla Glass 3" has been used in devices such as smartphones, tablets, notebook computers, and smartwatches. It is strong, thin and scratch resistant. Version 3 of this glass was developed in only 22 months, where four months were dedicated to the design stage, eight to the development stage, three months to the manufacturing stage, and finally seven months to the deployment stage. For each stage, a workflow is provided and one has to justify why and how materials modelling was an "accelerator", i.e. enabled the completion of a particular task of the workflow faster. Table 1Table 2 is a simplified, summarised version of a QBTM analysis, and ideally, an organisation should enhance this analysis by assessing how much costs and time could be saved with using modelling as opposed to previous workflows. Also, inhibitors should be listed, i.e. events that may slow the work and add costs. It may also be beneficial to set it up with a Gantt chart, similar to Figure 2 in the Gorilla Glass case study (NIST, Gorilla Glass, 2016).

Table 2: QBTM for Corning's Gorilla Glass

Corning	**Duration/ months**	**Summary of work**	**Materials Modelling as accelerator, because …**
Stage 1 Design	4	1. Establishment of Customer Target **2. Development of performance models based on topological constraint theory and existing databases** **3. Coupling of models for performance and manufacturing with cost modelling**	**Stage 1, point 2:** Availability of models as a function of glass composition Committed effort in fundamental research that provides high quality data as well as models **Stage 1, point 3:** ICME approach utilizing physics-based, "best available" models

Stage 2 Development	8	**1. Model composition melted and manufactured in production-scale tank** 2. Statistical “red flag” testing of product to determine product attributes 3. Sampling of product to customers for testing **4. Establishment of Ion Exchange (IOX) parameters at third party glass finishers**	**Stage 2, point 1:** Empirical modelling of the effects of composition on formation of fusion line zirconia defect **Stage 2, point 4:** Available models for the ion exchange processability
Stage 3 Manufacturing	3	1. Production of new composition in additional production-scale melting facilities in Corning network 2. Developed procedures for tank start-up and glass composition transition to improve long term manufacturability	N/A
Stage 4 Deployment	7	**1. Adjusting product to customer needs based on specific device design**	**Stage 4, point 1:** Device level modelling

Generally, in the Corning case, the breadth of data and models available as a result of the company’s strong and ongoing commitment to fundamental research served as an accelerator. For example, the availability of models enabled Corning to more quickly determine which materials compositions could best meet the specific customer requirements identified. Also critical to the efficiency of this stage was the use of an approach that incorporated materials design for performance with manufacturing-related and cost models. In future, this could be handled by a BDSS. For Corning, this integrated computational materials Engineering (ICME) approach was effective in identifying candidate compositions for production.

QuesTek applied materials modelling for developing Ferrium® M54® steel for application in U.S. Navy hook shanks. They provided a notable materials innovation for a structure-critical aerospace product. The time frame was much longer and 16 months were dedicated to the design stage, 28 to the development stage, 52 months to the manufacturing stage, and finally 16 months to the deployment stage. Table 3 shows a simplified, summarised version of a QBTM analysis.

Table 3: QBTM for QuesTek Ferrium® M54® steel; only tasks, that could be accelerated by modelling are listed.

Corning	Duration/ months	Summary of work	Materials Modelling as accelerator, because …
Stage 1 Design	16	**1. Concept generation** **2. Computational alloy design**	**Stage 1, point 1+2:** Proprietary Questek databases and QuesTek computational modelling capability
Stage 2 Development	28	**1. Sensitivity analysis and design**	**Stage 2, point 1:**

(8 months overlap with Stage 1)t			QuesTek “design for scale” modelling capabilities
Stage 3 Manufacturing	52	**1. New forging tool available with partner SIFCO Industries Inc., forging of 5 hook shanks**	**Stage 3, point 1:** simulation capability; learning from forging S53 in the past, SIFCO deform modelling enabled forging process modifications to obtain desired microstructure
Stage 4 Deployment	16	**N/A**	N/A

QuesTek generated and computationally designed materials that could potentially meet the specified requirements for the hook shanks. Besides their modelling capability, QuesTek profited from their proprietary databases. The combination of data and modelling were significant accelerators in discovering set of prospective alloy compositions. Development stage was supported by QuesTek’s “design for scale” modelling, which supported the casting process as well as the subsequent thermomechanical processing needed to produce a pilot material form suitable for mechanical property evaluation. In the manufacturing stage, SIFCO, a forging supplier, provided flow stress data to assist in forging modelling, which proved to be a key accelerator for this stage.

2.2.2. MGI Economic Analysis

To stress the importance materials modelling in industry, QBTM was used as a framework for a major study of typical durations, costs and success rates of each of the stages, comparing an ‘as is’ with a potential ‘to be’ scenario (Scott, Walsh, Anderson, O'Connor, & Tassey, 2018). The data required for this economic analysis were based on interviews with 121 experts from a range of chemicals, materials and manufacturing industries, most of whom worked in industry or were involved in industry projects. We will refer to this study in the following as the “MGI Economic Analysis”.

Considering Integrated Computational Materials Engineering (ICME) more widely, a range of factors have to be put in place to improve manufacturing and materials industry. The MGI Economic Analysis states these ‘needs’ (i.e. potential accelerators) as listed in column one and two of Table 4. We propose in the last column of Table 4 to classify these into four dimensions on which organisation can have an influence and which can provide means for acceleration and higher success: People, Tools, Process and Data. The maturity of organisations relative to these dimensions will be further analysed in Chapter 5.

Table 4: Accelerators and their classification into organisational dimensions

Causal Factor	Details	Dimension
Access to High-Quality Data	Non-proprietary experimental data, computational data, metadata, and software code	**DATA**
Collaborative Networks	Efficient means of sharing materials information (e.g., along a supply chain, among research collaborators)	**PEOPLE**
Material Design Methods	Enabling application of a systems approach to materials development, from discovery	

	and design all the way through to deployment	**PROCESS**
Production & Scale-Up	Model-based alternatives to expensive physical testing, trial and error–based approaches Faster, cost-effective means of producing advanced materials at pilot and full scales	**PROCESS**
Quality Assurance, Quality Control & Component Certification	Ability to model, predict, and control formation of defects Ability to forecast manufacturing variation	**TOOLS**
Model Validation & Uncertainty Quantification	Basis for trust and acceptance of computational models Basis for objective decision-making regarding reliance on computational analysis and simulation at a business level.	**TOOLS**

One of the major outcomes was that Materials Modelling and all other accelerators are expected to reduce the time to market by 3-5 years (Figure 7: Project Duration split into individual stagesFigure 7). The design stage duration profits most from acceleration and can be reduced by 46%. All other stages can be reduced by about an average of 30% each.

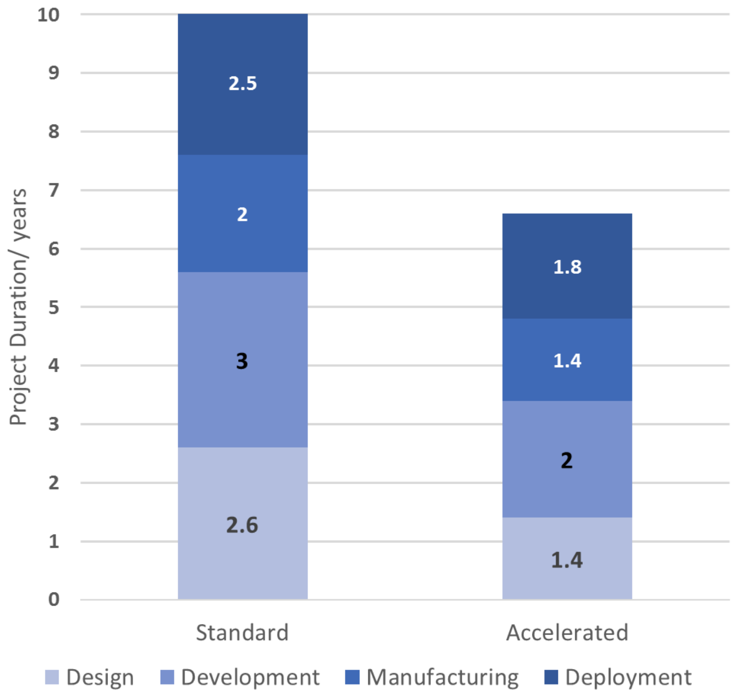

Figure 7: Project Duration split into individual stages, adapted from (Scott, Walsh, Anderson, O'Connor, & Tassey, 2018). Standard refers to normal conditions, and Accelerated to where modelling and other factors have been considered, i.e. a new infrastructure.

The relative cost of a project is depicted in Figure 8 normalised in units of "one design stage". This means if an organisation spends 1 monetary unit on design, the development stage costs 3.9 times as much, etc. In a standard environment, manufacturing and deployment stages are estimated to be, respectively, roughly four times and three times more cost-intensive than the development stage. Addressing the needs outlined in Table 4 is estimated to reduce relative costs by an average of 25% in the discovery/design stage.

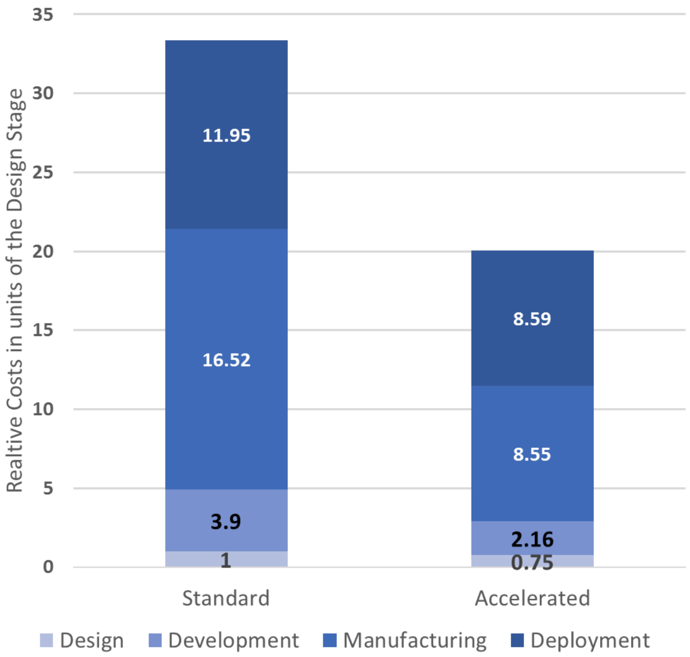

Figure 8: Relative Costs per stage in units of one Standard Design Stage, adapted from (Scott, Walsh, Anderson, O'Connor, & Tassey, 2018). Standard refers to normal conditions, and Accelerated to where modelling and other factors have been considered, i.e. a new infrastructure.

The stages where one can expect the most reduction of costs are development and manufacturing, with 45 and 48%, respectively.

Equipped with this evidence that materials modelling and related factors make a significant impact, an organisation should try to "reverse roadmap" successful projects using QBTM considering factors in all four dimensions: people, tools, process and data. We term this scheme "Four Dimensional QBTM" (4D-QBTM). As QBTM aligns very well with the macro and business process levels, it can serve as vehicle to communicate materials modelling impacts to higher levels of an organisation and be a basis for strategic planning and investment decisions.

Revisiting the Corning case on the basis of 4D-QBTM we could potentially identify more acceleration points and also improve the understanding of how all four dimensions play a role. The following section is a hypothetical exercise and shall not diminish the excellent case study Corning provided.

Table 5: Corning Case revisited with 4D-QBTM

Corning	Materials Modelling as accelerator, because …	4D-QBTM
Stage 1 **Design**	**Stage 1, point 2:** Availability of models as a function of glass composition Committed effort in fundamental research that provides high quality data as well as models **Stage 1, point 3:** ICME approach utilizing physics-based, "best available" models	**PEOPLE:** Corning has access to modellers **TOOLS:** Corning has physics-based models **PROCESS:** IMCE approach **DATA:** high quality data are seen as a "must-have"
Stage 2 **Development**	**Stage 2, point 1:** Empirical modelling of the effects of composition on formation of fusion line zirconia defect **Stage 2, point 4:** Available models for the ion exchange processability	**PEOPLE** are using **TOOLS** very well. What 4D-QBTM can add is answers to questions: How is this process of tool usage documented (**PROCESS**) and where are the **DATA** resulting from this process going? Adding **PROCESS** and **DATA** management plan could accelerate a future development process
Stage 3 **Manufacturing**		What value 4D-QBTM can add is how to get more modelling into the actual manufacturing stage to questions: Do you have **PEOPLE** and **TOOLS** that could interact with your vertical supply chain? What **PROCESS** do we need and what **DATA** can be used or gained?
Stage 4 **Deployment**	**Stage 4, point 1:** Device level modelling	Corning has **TOOLS** and **PEOPLE** and **DATA** to permit device level modelling and thus, accelerate the Deployment stage. 4D-QBTM would ask to uncover the **PROCESS** behind and enable stakeholders to streamline and capture the device modelling better.

Hence, 4D-QBTM would attempt to strengthen existing modelling accelerators and make sure all four dimensions play a strong role. For each of the four stages an assessment should be made to determine the status quo and see what else is needed to accelerate each stage. The resulting 4D-QBTM methodology is illustrated in Figure 9.

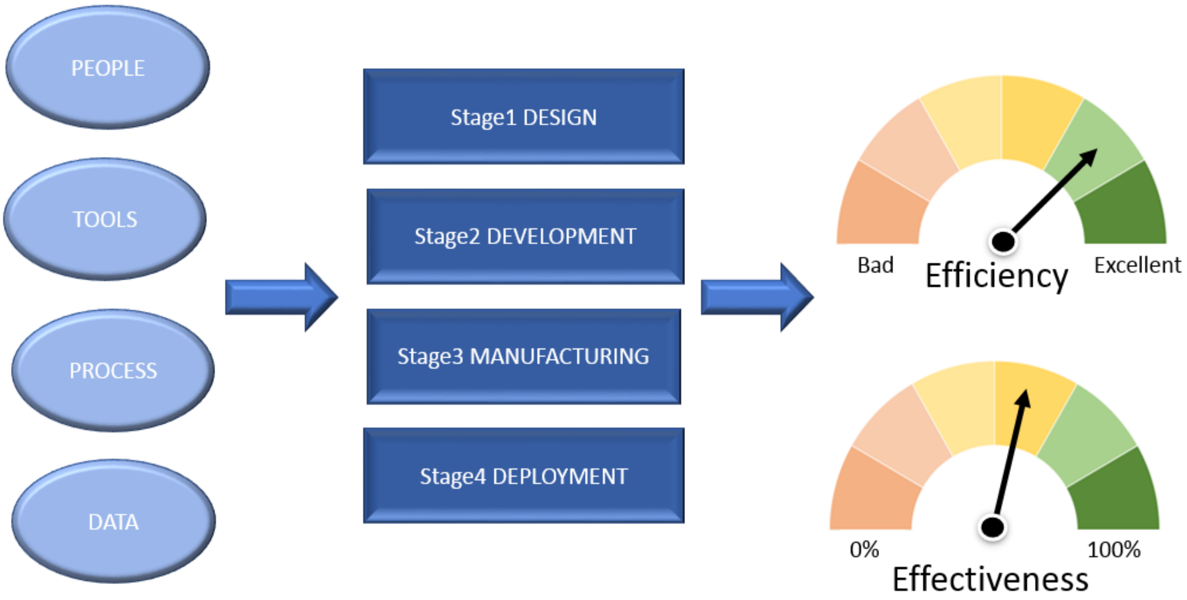

Figure 9: Four dimensions, four stages, and efficiency/effectiveness gauges

The decision makers assign people, tools, process and data as resources to activities and tasks at each of the four stages. To check if the deployment was successful for each stage, they define KPIs measuring the efficiency and the effectiveness. KPIs for efficiency could be duration of a stage, and a KPI for effectiveness could be percentage of materials candidates that successfully passed on to a next stage.

With an improved infrastructure, materials R&D projects are more likely to transition from a design state to successive stages. In general, the RTI study (Scott, Walsh, Anderson, O'Connor, & Tassey, 2018) found that currently about 1 out of 10 projects survives all stages (Figure 10). With improved infrastructure, 1 out of 5 projects can be expected to move to the last stage, hence, a 20% chance of deployment with improved infrastructure versus a 10% chance. The number of projects that must enter the development stage for every one that reaches the deployment stage improves from 2.9 to 2.1 (a 48% chance of deployment, conditional on reaching the development stage, with improved infrastructure versus a 35% chance currently).

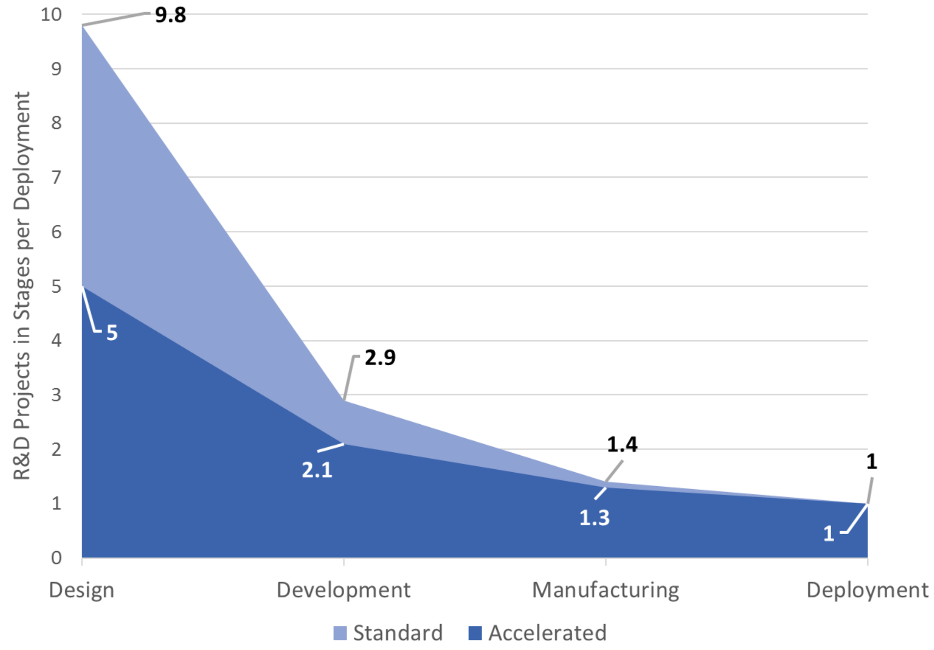

Figure 10: Potential Impact on Deployment Risk, adapted from (Scott, Walsh, Anderson, O'Connor, & Tassey, 2018)

Overall, estimated potential impacts of an improved Materials Innovation Infrastructure achieve a 71% improvement in R&D efficiency. Here R&D efficiency is the percentage reduction in average R&D investment cost per new material deployed.

2.2.3. Out-of-Pocket and Capitalised Costs

The MGI Economic Analysis also provides the so-called out of-pocket cost and capitalised costs for each of the stages. This sort of costing has on often been used in R&D cost analysis for the pharmaceutical industry, for example see (DiMasi, Grabowski, & Hansen, 2016).

Out-of-pocket costs are given by:

$$C(t_{start} - t_{end})/p$$

Equation 1: Out-of-pocket Costs (Scott, Walsh, Anderson, O'Connor, & Tassey, 2018)

Where c is the cost per year per project for that stage, t_{start} is the time from the start of the stage to the end of the deployment stage, t_{end} is the time, in years, from the end of the stage to the end of the deployment stage, and p is the probability of deployment, conditional on reaching the stage. The values for each stage are provided in Table 6.

Table 6: Parameters needed for out-of-pocket and capitalised cost calculations for all stages with standard and accelerated conditions, values taken from Chapter 3 of (Scott, Walsh, Anderson, O'Connor, & Tassey, 2018)

	Standard				Accelerated			
STAGE [a]	**1**	**2**	**3**	**4**	**1**	**2**	**3**	**4**
c **Cost per year per project in that stage [b]**	1.0	3.90	16.52	11.95	0.75	2.16	8.55	8.59
p **Probability of deployment, conditional on reaching the stage/%**	10	35	72	100	20	48	77	100
Duration/year	2.6	3	2	2.5	1.4	2	1.4	1.8
t_{start}/years	10.1	7.5	4.5	2.5	6.6	5.2	3.2	1.8
t_{end}/years	7.5	4.5	2.5	0.0	5.2	3.2	1.8	0.0
Out-of-pocket Cost [c]	26.0	33.4	45.9	29.9	5.3	9	15.5	15.5
Capitalised Cost [c]	51.3	53.2	60.1	32.9	8.3	12.4	18.9	16.6

[a] 1 Design, 2 Development, 3 Manufacturing, 4 Deployment

[b] in units of one standard design year

[c] compared to (Scott, Walsh, Anderson, O'Connor, & Tassey, 2018), there may be rounding errors.

Thus, to calculate the out-of-pocket cost for the standard design stage we need

$$1 * \frac{10.1 - 7.5}{0.10} = 26.0$$

Equation 2: Out-of-pocket cost using parameters of standard Stage1 (Design), see Table 6

One can see that an accelerated version of the four stages leads to out-of-pocket cost reduction of 80% for the design stage, 73% for the development stage, 66% for the Manufacturing stage and 50% for the deployment stage.

Another relevant cost to look at is the capitalized cost,

$$\frac{c \int_{t_{end}}^{t_{start}} e^{rt}\, dt}{p} = c(e^{rt_{start}} - e^{rt_{end}})/pr$$

Equation 3: Capitalised costs (Scott, Walsh, Anderson, O'Connor, & Tassey, 2018)

Where the new parameter r is the real cost of capital, as a continuously compounded annual rate. (Chen, 2019). Assuming an 8% cost of capital this is converted to a continuously compounded annual rate via r=ln(1.08)=0.077 or 7.7%.

Thus, to calculate the capitalised cost for the standard design stage we need

$$1 * \frac{e^{0.077*10.1} - e^{0.077*7.5}}{0.1 * 0.077} = 51.3$$

Equation 4: Capitalisation Cost using parameters of standard Stage1 (Design), see Table 6

An accelerated version of the four stages leads to a capitalised cost reduction of 84% for the design stage, 77% for the development stage, 69% for the Manufacturing stage and 50% for the deployment stage.

2.2.4. Return on Investment (ROI)

ROI is useful for reviewing and tracking performance for materials modelling functions as a whole, since on the investment side, all investments need to be incorporated (employees, training, software and hardware, …) and on the return side all types of returns including cost savings, faster to market, increased revenue etc.

A simple ROI can be defined as the ratio of the overall revenue generated from a product that was developed with the support of modelling and the cost of the modelling project:

$$RoI = \frac{Revenue\ generated\ from\ project}{Modelling\ investement\ in\ project}$$

Equation 5: "Simple" ROI

This metrics was used in a previous Materials Modelling Impact study (Goldbeck & Court, The Economic Impact of Materials Modelling, 2016). This study reports that out of 29 interviewed companies about 80% reported innovation accomplishment, 60% cost savings, 35% job creation, and 30% revenue increase due to materials modelling. The “simple” ROI ranged from 2 to 1000 and removing the most extreme largest and smallest values, an average of 8 was found.

A study performed by IDC (Swenson, Languell, & Golden, 2004) for Accelrys Inc.[1] used a more elaborate way of ROI.

$$RoI = \frac{B}{C}$$

Equation 6: "Detailed” ROI

Where B is the quantified benefit attributed to modelling and C is the cost of modelling. The Benefit in Equation 6 is calculated as

$$B = Vt_{mechanism} \times Np_{cost} \times R_{cost}$$

Equation 7: Quantified benefit attributed to modelling

Where:

$Vt_{mechanism}$ is the total value of the respective impact mechanism (more efficient experimentation, broader exploration and deeper understanding, saving a product development project and/or accelerated product development etc.)

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[1] Now Biovia, Dassault Systemes.

Np_{cost} is the Number of projects that involve modelling, which is a function of the resource available, hence cost.

R_{cost} is the 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 Cost in Equation 6 is calculated as

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

Equation 8: Cost attributed to modelling

Where SW is the Software cost, HW is the Hardware cost, IT is the IT support cost, L is the Labour cost and T is the Training cost.

Using the detailed ROI, the IDC report suggests a cumulative ROI in the range of 3 to 9, where use of more expert (rather than occasional) users is associated with higher ROI. A detailed ROI elaboration for these scenarios as well as a typical ROI based on updated figures for software and hardware costs etc can be found in a White Paper (Goldbeck, 2012).

Similarly, another IDC report estimated the ROI of materials modelling in pharmaceutical development and formulation, based on the two key scenarios of improved efficiencies and product development saves and arrived at the following figures:

- ROI (Improved efficiencies) = 2.7 (low investment), 7.0 (high investment)
- ROI (Product Development Saves) = 0.4 (low investment), 2.8 (high investment)
- TOTAL ROI = 3.1 (low investment), 9.8 (high investment)

Concerning the apparently higher impact of expert modellers it should be noted (a) since this study was carried out, the range of tools applicable to the occasional user has increased and (b) that every organisation needs an appropriate balance of breadth and depth and (c) as will be discussed below, organisations with a high maturity consider a range of modelling roles, including translators. Note that the IDC studies did not take into account the effect of experts providing translation and workflows to occasional users and thereby broadening the impact.

2.2.5. Net Present Value (NPV)

Embarking on materials modelling requires acquisition of software. NPV is useful for assessing for the value of investing in a particular type of software (Irani, Ezingeard, & Grieve, 1997). It is also a relatively widely used measure (together with Internal Rate of Return, IRR) for management decisions about R&D projects, hence in many companies the methodology already exists. A given scenario is considered economically beneficial if it has the highest IRR and the NPV is greater than zero.

The NPV is the difference between the present value of cash inflows and the present value of cash outflows over a period of time (Kenton, W., 2019) and it indicates, how much value a project adds to an investment.

$$NPV = \sum_{t=1}^{n} \frac{R_t}{(1+i)^t}$$

Equation 9: Net Present Value

where:

- R_t is the net cash inflow- outflow (difference between revenues and expenditures) during a single time period, t
- i is the discount rate or a return that could be earned if the cash was invested alternatively

An excellent illustration of the use of NPV for the assessment of whether to deploy simulations to support for specific Activities (Level 4 processes) was presented by (Am Ende, Hancock, & Huta, 2010). The challenge was to establish if materials modelling can aid to decrease the number of experiments in pilot scale trials and to eliminate the need to produce one or more expensive, commercial-scale batches during development.

The costs associated with modelling were software licenses, number of full-time employees (FTEs) and hardware costs. To move a project from laboratory to pilot scale the cost around the active pharmaceutical ingredient (API), FTEs, lab supplies, costs of batches at the pilot and commercial scales (during development studies) need to be considered.

Table 7: NPV of Drug Product Computational Approaches compared to costs, adapted from (Am Ende, Hancock, & Huta, 2010)

Application	Cost/$k	1 Yr Value/$k	3 yr Value/$k
Powder Mixing and Lubrication	28	1,970	6,740
Drug Product Formulation Design	7	75	225
Film Coating	79	495	1,710
Wet Granulation	2	325	975
Drug Product Milling	9	80	275
Process Control	5	0[a]	17
Material Handling	47	1,070	3,390
Tableting	49	4	72
Capsule Filling	66	15	43

[a] Process Control has no benefit in the first two years.

Table 7 shows that the areas with the greatest projected value are Powder mixing, Material handling and Film coating. Tableting would not profit from modelling and should hence be put on hold until improved software tools emerge on the market.

2.2.6. Total Cost of Ownership (TCO)

Any of the quantitative tools outlined above requires a good understanding of the cost side of deploying modelling, including staff (and their training), hardware and related infrastructure as well as software. To aid decisions about the software, a Total Cost of Ownership (TCO) calculation can be helpful (Ellram, 1995). As outlined in a blog post about “Deciding between Open Source and Proprietary CFD software”, (Stephens, 2016) TCO refers to all the costs associated with the use of computer hardware and software. This would include administration, licencing, hardware and software updates, training and development, maintenance, technical support and any other associated costs. Total cost of ownership analysis can serve as a planning and decision-making tool in itself as well as support ROI calculations.

3. Benefits Management

The focus of the previous sections has been how materials modelling impacts on typical Key Performance Indicators of Activities, Sub-Processes and Processes in an enterprise, such as Stage duration, cost and probability of success as well as ROI and NPV, i.e. monetary measures quantifying the value of certain investments.

However, it is important not to lose sight of the multi-dimensional nature of factors that play a role, hence our introduction of the 4D-QBTM, and the multitude of potential areas that can be influenced by the introduction and wider use of a technology such as materials modelling.

The EMMC[2] therefore looked into identifying what benefits could emerge for an organisation when using modelling. The following is a collection of benefits that have been identified in a number of studies (Goldbeck & Court, The Economic Impact of Materials Modelling, 2016) (Swenson, Languell, & Golden, 2004) and direct interactions with industrial end users.

3.1. What are the Benefits?

Using the levels described in Figure 1, we can associate the following benefits to each level:

Level 1: Macro

- R&D strategy development, e.g. via early exploration of behaviour in downstream applications
- Support broader IP claims.
- Support defensive IP publishing, i.e. pre-empt competition patents.
- 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.
- Improve value chain interactions
    - Validation of supplier information
    - Build customer trust
    - Demonstrate competitive advantage via competitor materials based on models
- 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)
- Communication and marketing via models and their visualisation

Level 2: Business Process

- Improved, deeper insight and understanding, hence:
    - Avoid dead-ends in R&D
    - Ability to link materials chemistry/structure to application performance
    - Enables better informed decisions about material, product and processing choices
    - Avoid upscaling issues and lower risk of market introduction; reduction of product failures during manufacturing, and after manufacturing

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[2] https://emmc.info/business-benefits-and-key-performance-indicators-kpis-of-materials-modelling/

    - Support trouble-shooting of material/product failures
- Design innovation and quicker identification of materials.
- Improved capabilities for predicting engineering system performance or life cycle.

Level 3: Sub-Process

- More efficient and targeted experimentation, saving time and cost of experiments
- Broader exploration
- Faster optimisation of material, formulation and/or process
- Fail early, innovate faster
- Solutions to design problems.
- Faster and less costly new product development.
- Better control of the manufacturing process.
- Faster time-to-market for new products.
- Support digitalisation

Level 4: Task

- Avoiding potentially hazardous experimentation
- Lower cost to obtain certain property data (e.g. due to cost of experiment or synthesis)
- Estimate property data for materials that cannot be obtained for competitive reasons.
- Solve problems which could otherwise not be solved
- Avoid destructive testing.
- Virtual engineering assessment of new materials that might be considered risky to assess with physical prototypes.
- Virtual engineering assessment in systems where the validation of materials performance by system-level testing is expensive, time consuming, or not possible.

3.2. How to manage the realisation of these benefits?

As we have seen, there is a plethora of potential benefits that modelling can bring. However, in order to ensure that an organisation realises these benefits, pro-active benefits management is required. A process model for benefits management, adapted from (Ward & Daniel, 2006) is depicted in Figure 11.

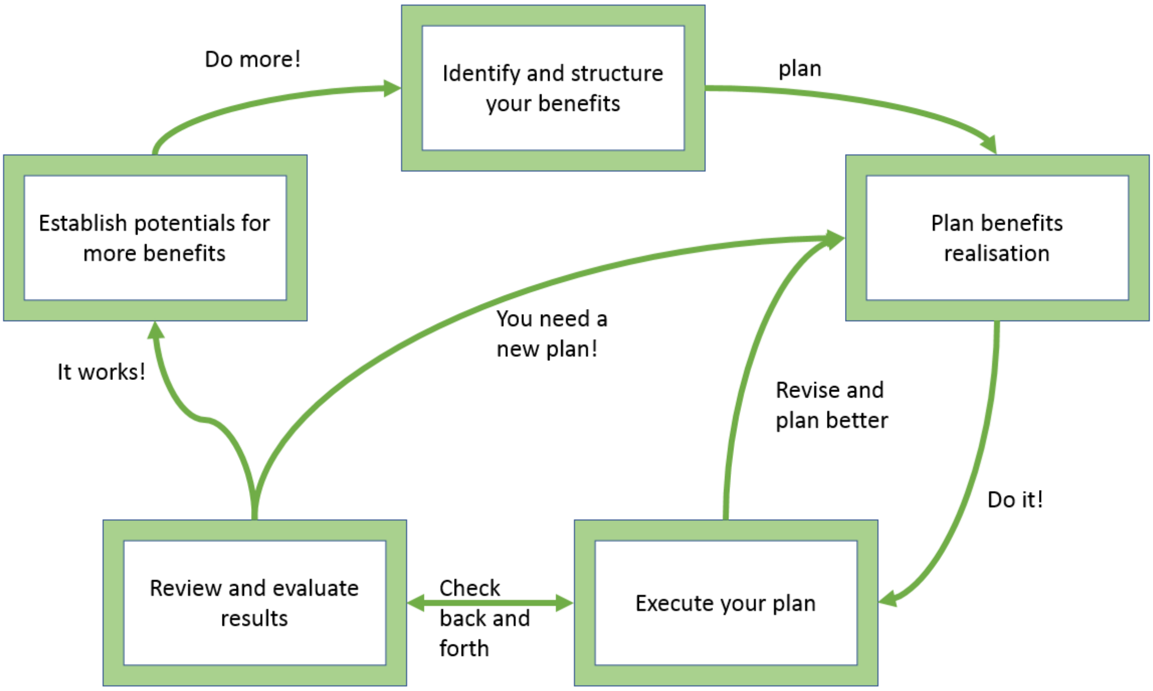

Figure 11: A process model for benefits management, adapted from (Ward & Daniel, 2006)

The first step is the identification of target benefits. For example, you want to bring "Quicker identification of materials" as benefit to your organisation. You have realised that "Quicker identification of materials" is beneficial for your organisation as you could beat the competition and bring your product faster to the market. You need to make sure, that your organisation actually wants this benefit and that you can improve an existing process. Your organisation will want to know if your proposed benefit can be measured, quantified and has a (financial) value. You then can take ownership and do a 4D-QBTM analysis to show that materials modelling (in its four dimension) can indeed play a role to realise this benefit. You also can argue here why you require more people, tools, processes and data to achieve this benefit. You may also have to revise your plans and plan differently if you have a lack in (or less mature) materials modelling dimensions. As you can see above, you will have to bring changes to your organisation: "*If you want something new, you have to stop doing something old*"[3] Benefits go hand in hand with changes (Ward & Daniel, 2006), and you have to state whether you do new things, do things better or stop doing things and how it relates to the benefit you target.

Additionally, you should consider a benefits dependency network[4], as depicted in Figure 12.

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[3] By Peter F. Drucker

[4] http://www.open.ac.uk/business-school/sites/www.open.ac.uk.business-school/files/file/corporate/Benefits_Management_29_Nov_12.pdf uses a booking tool for the UK National Health Service as an illustrative example how to work out a benefits dependency network.

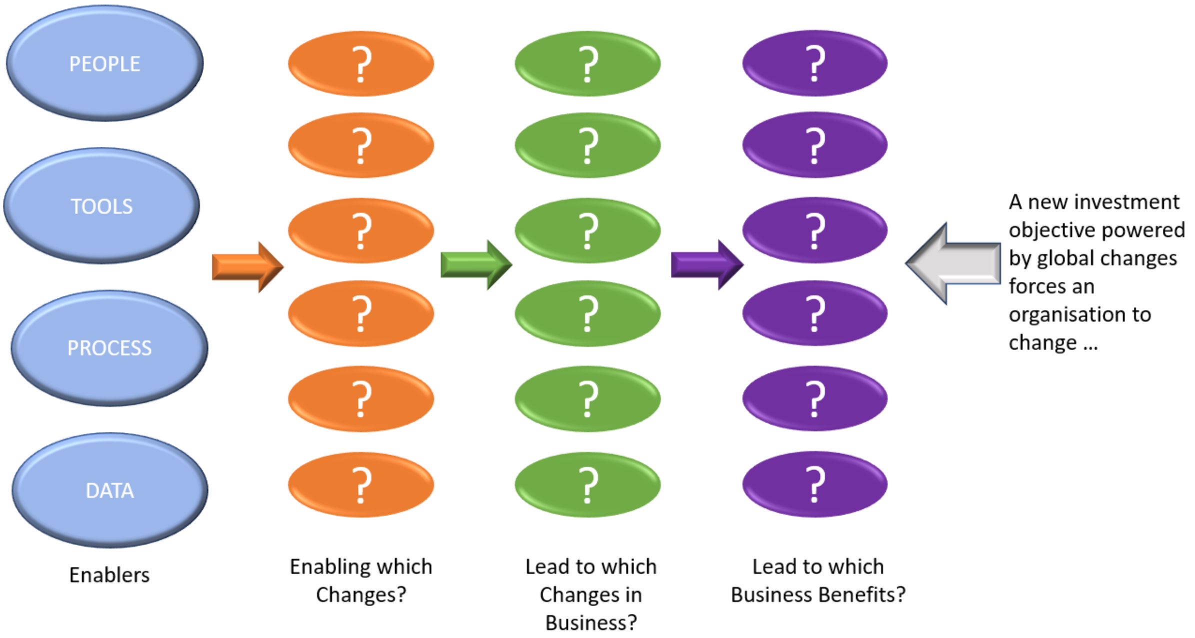

Figure 12: A benefits dependency network, adapted from (Ward & Daniel, 2006)

What really will drive an organisation to adopt benefits management are the challenges of today's world such as shifts in global economic power, rapid urbanisation, resource scarcity, etc. (Lahmann, Probst, & Parlitz, 2019) will rapidly force organisations to address change. The authors of this white paper state: "*Due to these global economic drivers, organisations have to question their existing set-ups and transform themselves, resulting in a comprehensive change in strategy, operating model, structure, people and processes where appropriate*". Investing in people, tools, process and data will generate the enablers quite naturally, and Chapter 4 will investigate how mature these enablers actually are and in Chapter 5 we will discuss, if unleashed to their full potentials, which "Enabling Changes" can and should be made. Enabling Changes means "doing new things" and the benefits dependency network should list which changes are needed. Importantly, the change needs to be connected to business benefit, so that an ROI can be determined.

Once all is in place you may want to evaluate and review your plans and check if your proposed "new things" are performing well, i.e. they are focussed, appropriate balanced, robust, integrated and cost effective. (NAO, 2001). Table 8: The characteristics of good benefits, adapted from offers possible solutions:

Table 8: The characteristics of good benefits, adapted from (NAO, 2001)

Criteria	Explanation	You can ...
Focussed	organisation's aims and objectives	Follow your organisations KPI's
Appropriate	Stakeholders who are likely to use it	Provide workflows for your colleagues to a standard that is deemed "appropriate"
Balanced	Does your benefit affect many stakeholders in your organisation and how?	Provide acceptance criteria for stakeholders to make sure you implement your changes in an acceptable way.
Robust	Withstand organisational changes or individuals leaving	Put a process in place and document your changes

Integrated	Being part of the business planning and management	Provide translation [a] and 4D-QBTM
Cost Effective	Balancing the benefits against the costs	Provide ROI, NPV, etc.

[a] (Hristova-Bogaerds, et al., 2019)

3.3. Benefit management in modelling projects

An illustrative example of pro-active benefits management comes from a study in the field of computer assisted drug design (CADD) carried out at Bristol-Myers Squibb (Loughney, Claus, & Johnson, 2011). Benefits management involved tracking the performance of a CADD team, a group that could be classified as “knowledge workers” (Drucker, 1969) and not very amenable to any sort of metrics. Without taking away the native creativity unique to such projects it was possible to design an outcome-oriented metrics to track and assess performance and steer behaviour towards realising more impactful projects.

Bristol-Myers Squibb defined three levels of impact:

- Level 1: Provision of data from modelling to other functions in the organisation.
- Level 2: The data triggered a response action that led to consistent results, for example characterised and/or synthesized a compound that showed the effects indicated by the model.
- Level 3: Project leader agrees in writing that modelling made an essential contribution to the project progress. (Would not have progressed without it).

The impact levels, including data, analysis, scientific decision support, and programme impacts are also shown graphically in Figure 133, which is adapted from (Loughney, Claus, & Johnson, 2011) for the case of materials modelling. At Level 1, data are provided to an R&D programme, followed by analysis. At Level 2, the information provided by modelling has an impact on individual steps in an R&D process. This in itself typically leads to cost and time saving. At Level 3, modelling has led to improvements in the overall outcome such as a new/improved material, process or component.

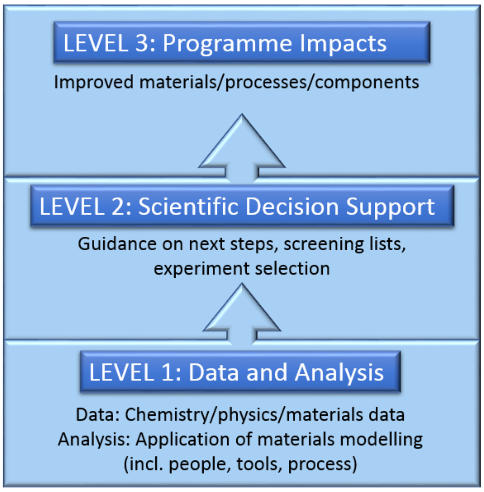

Figure 13: Levels of Impact as identified for CADD and adapted for Materials Modelling.

In the case example reported by Bristol-Myers Squibb, the impact metrics exercise led the organisation to use its resources more efficiently and effectively. The number of projects where no contributions could be made fell while there was a strong rise in projects with Level 2 and Level 3 impact over a four-year period.

This increased focus meant for the modellers that "nice to have" modelling requests could be avoided and as a metrics was in place, they could easily evidence whether a project had an impact or not. They also became more visible and this permitted their superiors to think strategically about resources.

4. State of industry: Maturity of materials modelling

4.1. Introduction to Maturity Models

Realising the benefits of modelling consistently, repeatedly and pervasively throughout an organisation requires a high level of maturity of the management and use of the technology. Maturity models (Schumacher, Erol, & Sihn, 2016) are suitable as a benchmarking framework and they can help organisations to improve their performance. Ideally, they are set out to enable an objective mapping of "as is" and "to be" states for business activities and operations.

For example, the Capability Maturity Model Integration (CMMI) (CMMI Product Team, 2002) is a process level improvement and appraisal programme which was originally developed to provide guidance for improving processes that meet the business goals of an organisation. It distinguishes five maturity levels as shown in Figure 14:

- Initial: indicates processes are unpredictable, poorly controlled and reactive
- Defined: Processes are characterised for projects but are often reactive
- Integrated: Processes are integrated in the organisation and are proactive
- Managed: Processes are measured and controlled throughout the organisation
- Optimised: Characterised by continuous process improvement

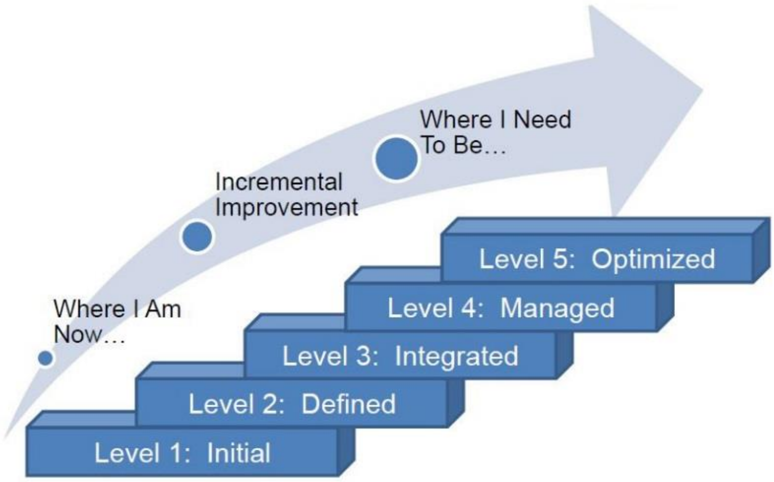

Figure 14: The levels of maturity and how to move forward

Considering the above definitions, it also becomes evident that a technology needs to reach a certain level of maturity in order to infiltrate high enterprise level processes, as indicated by the ladders in Figure 15.

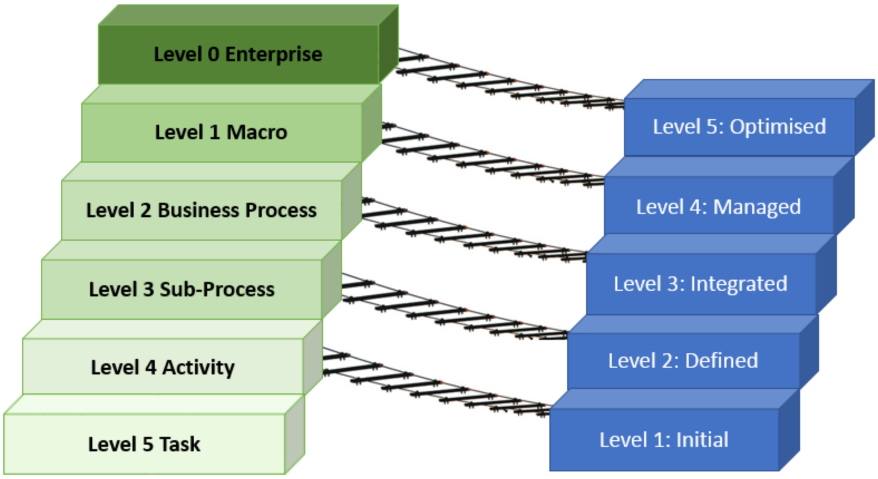

Figure 15: Business Process levels adjoined with Materials Modelling Maturity Levels

4.2. Maturity Model for Materials Modelling

In order to support industry in assessing the maturity of their modelling activity and guide it to higher levels or maturity and hence impact regarding enterprise level processes, EMMC adapted a maturity model (Biovia, 2012) comprising five levels (Figure 16) developed by Accelrys[5]. Based on CMMI, the model has been tailored to scientific organisations. It establishes a maturity level mapping of characteristics and behaviours in each of the four dimensions discussed above for the 4D-QBTM: people, tools, data, and processes (Figure 16, *Table 9*).

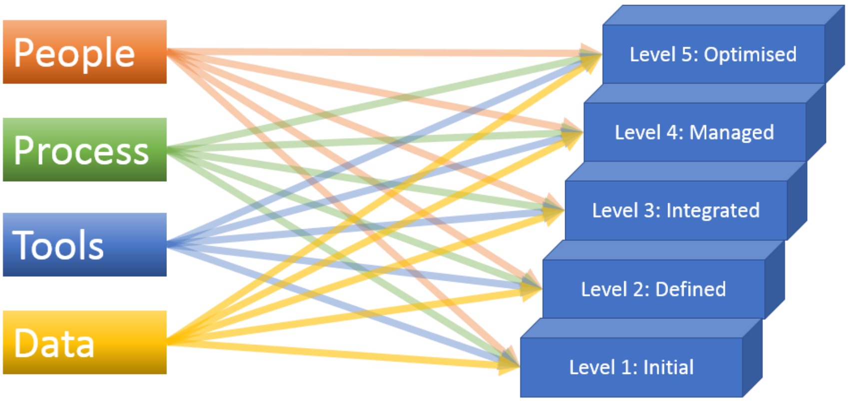

Figure 16: Mapping of characteristics and behaviours in each of 4 key areas to a "Level"

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[5] Now Biovia, Dassault Systemes.

- **People** relevant to materials modelling are different types of modellers, ranging from expert modellers to occasional users of modelling, experimental scientists that require modelling results e.g. for interpretation of analytical data, translators and other related stakeholders.
- **Processes** involve modelling workflows as well as more widely workflows at and across different stages of QBTM that involve modelling or data from modelling, translation of challenges into modelling options and the interaction of modelling with wider projects and the organisation as a whole.
- **Tools** cover software and hardware, their selection and use and their connections with other IT systems.
- **Data**, includes storage and handling (security, access, provenance, persistence), but also how the information is managed. In fact, all aspects that apply to FAIR data should be applied within an organisation.

Table 9 provides descriptions of each maturity level with respect to each of the dimensions.

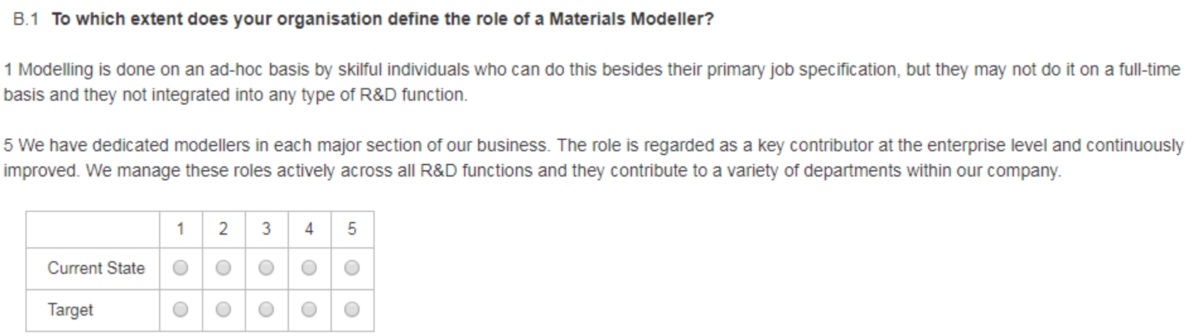
Table 9: Maturity Model dimensions and their manifestation on different levels

Maturity	People	Process	Tools	Data
Initial	Isolated expertise and knowledge Reliance on individuals Source of value and power	Based on individual skill and choice Highly variable	Acquired based on individual preference Not integrated with other tools and systems	Ad hoc storage
Defined	Expertise and knowledge shared within function, lab or department but not beyond Departmental collaboration & training	Consistency within teams Translation acknowledged but not widely shared	Validated tools but with some inconsistencies Different tools not well integrated No integration beyond modelling function	Data policies at departmental level Lack of integration across organisation
Integrated	Collaboration across science and business functions; backed up by policies, integrated objectives	Well documented and accessible Consistently deployed and followed	Standards for selection and application Integrated platforms on a syntactic level	Data policies at organisational level Integrated information architecture
Managed	Consistent evaluation Performance objectives standardised	Integration into business workflows Traceable to specific models and workflows	Centrally managed Cross-domain interoperability Cross-functional workflow integration	Management of roles, security, provenance, Enables sharing along value chain Semantic
Optimised	Enterprise viewpoint Continuous improvement culture	Well documented and accessible Consistently deployed and followed Fully integrated in business decisions	Integrated platforms Fully integrated with semantic data systems	Timely, relevant and available Machine learning and AI integrated

4.3. Materials Modelling Maturity Self-Assessment

In order to support organisations in assessing their ‘as is’ and ‘to be’ levels of maturity in utilising materials modelling, EMMC designed an online questionnaire[6]. It serves both as a self-assessment tool and a means for EMMC to survey the field and get an insight into the state of the industry.

We formulated seven to eight questions probing aspects (individual ‘pillars’) of each of the four dimensions (Figure 17). Two answers are offered that represent the lowest maturity (1, initial) and the highest maturity (5, optimised) and participants are asked to rank their organisation on this scale from 1 to 5. The maturity for each dimension is obtained by averaging across these individual questions. In each case, both the perceived current maturity and the maturity targeted in 3-5 years was probed.



B.1 **To which extent does your organisation define the role of a Materials Modeller?**

1 Modelling is done on an ad-hoc basis by skilful individuals who can do this besides their primary job specification, but they may not do it on a full-time basis and they not integrated into any type of R&D function.

5 We have dedicated modellers in each major section of our business. The role is regarded as a key contributor at the enterprise level and continuously improved. We manage these roles actively across all R&D functions and they contribute to a variety of departments within our company.

	1	2	3	4	5
Current State	○	○	○	○	○
Target	○	○	○	○	○

Figure 17: Question 1 out of 8 for the dimension “People”. 2 answers representing the lowest and the highest maturity are provided as guideline and a tick box array permits to choose the current and the target maturity.

Finally, a set of ‘self-assessment’ statements for each dimension was presented, with five carefully formulated choices reflecting the levels of maturity (Table 10). All statements are formulated in a positive way as there is no “bad” level to be at; for example, there are many examples of highly successful applications of materials modelling at Level 1, typically relying on some highly expert modeller.

For each dimension, participants answered a number of dimension questions and chose an overall maturity level reflecting the status of their organisation. Comparison of average pillar assessment and overall self-assessment typically reflects pillars, i.e. aspects of maturity that are strongly above or below average.

Table 10: Self-assessment questions for each key area

Key Area	Question	Maturity Level
People	We have isolated expertise and knowledge; we rely on individuals.	Initial
	Expertise and knowledge are shared within function, lab or department but not beyond; There are departmental collaboration and training.	Defined
	There is collaboration across science and business functions which is backed up by policies and integrated objectives specifically for materials modelling.	Integrated

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[6] See Supplementary_Info_1.pdf

	There is a consistent evaluation of our modelling teams and all performance objectives standardised.	Managed
	Our modelling teams are at Enterprise viewpoint and we practice a continuous improvement culture.	Optimised
Process	Everything is based on individual skill and choice and thus, highly variable.	Initial
	There is consistency within teams and translation is an acknowledged skill but not widely shared.	Defined
	Our process is well documented and accessible and consistently deployed and followed.	Integrated
	We do have integration into business workflows and everything is traceable to specific models and workflows.	Managed
	Everything with respect to modelling is well documented and accessible, consistently deployed and followed and modelling is part of our business decisions.	Optimised
Tools	Our modelling tools are acquired based on individual preference and they are not integrated with other tools and systems.	Initial
	We do use validated tools but inconsistencies remain. All the different tools are not well integrated, files cannot be automatically passed on between them and there is no integration beyond the modelling function.	Defined
	We do operate standards for selection and application of tools and we have integrated platforms on a syntactic level.	Integrated
	Our tool acquirement process is centrally managed. All tools need to be cross-domain interoperable as we rely on cross-functional workflow integration.	Managed
	We operate on fully integrated platforms which are by themselves fully integrated with semantic data systems.	Optimised
Data	We operate ad hoc storage and have a lack of policies about data management.	Initial
	Each department has data policies but there is a lack of integration across our organisation.	Defined
	We do operate data policies at the organisational level and have integrated information architecture.	Integrated
	We have dedicated personnel, provenance, and security in place. This all enables us sharing along our value chains.	Managed
	Or data are timely, relevant and available. Machine learning and AI is fully integrated.	Optimised

4.4. The Materials Modelling Maturity – results

About 120 materials modellers in different industry sectors were approached to take part. Generally, interest was very strong and in many cases the results were deemed to be too business sensitive for sharing. Completed surveys were obtained from 16 different organisations on the proviso of anonymity. The sample reflects a range of industries, materials modelling methods and experiences with materials modelling. It includes two companies from the pharmaceuticals and fine chemicals field, nine companies from the specialty chemicals and materials field and five manufacturing companies. Four organisations used only or almost only continuum modelling, four used only discrete modelling (electronic, atomistic, mesoscopic) with the remaining eight using both types of models. The average maturity level results are presented in Figure 18.

In addition to the results gathered by means of the survey, EMMC conducted two workshops (25th of September 2018 in Cambridge and 16th of May 2019 in London) and a session at its Second International Workshop (25th – 27th February 2019 in Vienna) which provided further input.

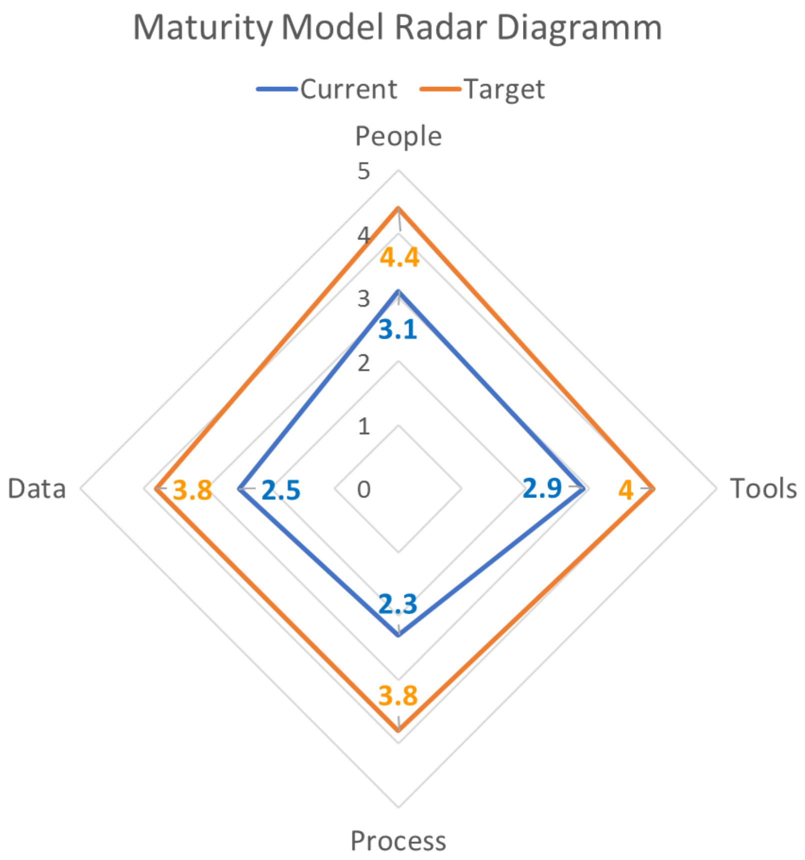

Figure 18: Current (blue ribbon) and target (orange ribbon) of Materials Modelling maturity: Initial (1), Defined (2), Integrated (3), Managed (4), Optimised (5)

It shows that the dimension "People" is most mature (average 3.1). It has reached an Integrated Level and organisations are very ambitious to reach a Managed Level as their target maturity is 4.4. This means, staff related to materials modelling can address sub-level business processes with a tendency to influence the actual business process (Figure 15). The dimension "Tools" is currently the second most mature (current maturity 2.9) and is moving from a Defined to an Integrated Level. With respect to a business process, tools are noticed on the sub-process level. Organisations would like to move beyond the Integrated level with a prospect to reach a Managed Level (target maturity 4.0). Data and Process, with a current maturity of 2.5 and 2.3, respectively, have reached a Defined Level. Organisations target the Process dimension (target maturity 3.8) to become as mature as the Data dimension (target maturity 3.8) over the next three years. Thus, data and process remain very much task and activity centred and are note much noticed on higher business levels.

4.5. Variations across organisations

There was no discernible difference between industry sectors for People, Process and Data maturity. However, in the Tools dimension, the average maturity in Manufacturing is 3.2 which is considerably above that of the Chemicals and Materials industry organisations (average 2.5). It may be related to the fact that some of the Manufacturing responses are from roles closer to engineering than R&D.

In terms of experience using materials modelling, seven organisations have less than ten years of experience, three are in the range of 10-20 years and four had more than 20 years. Our results show that maturity levels tend to increase with organisational experience of using materials modelling, as shown in Figure 19. The increase is particularly marked for the People and Process dimensions. One can speculate that Tools and Data are more driven by available software and IT systems while People and Processes maturity depends more on embedding materials modelling inside an organisation, which grows over time. Note that there was no discernible trend of maturity level as a function of the experience of the individual modellers in an organisation.

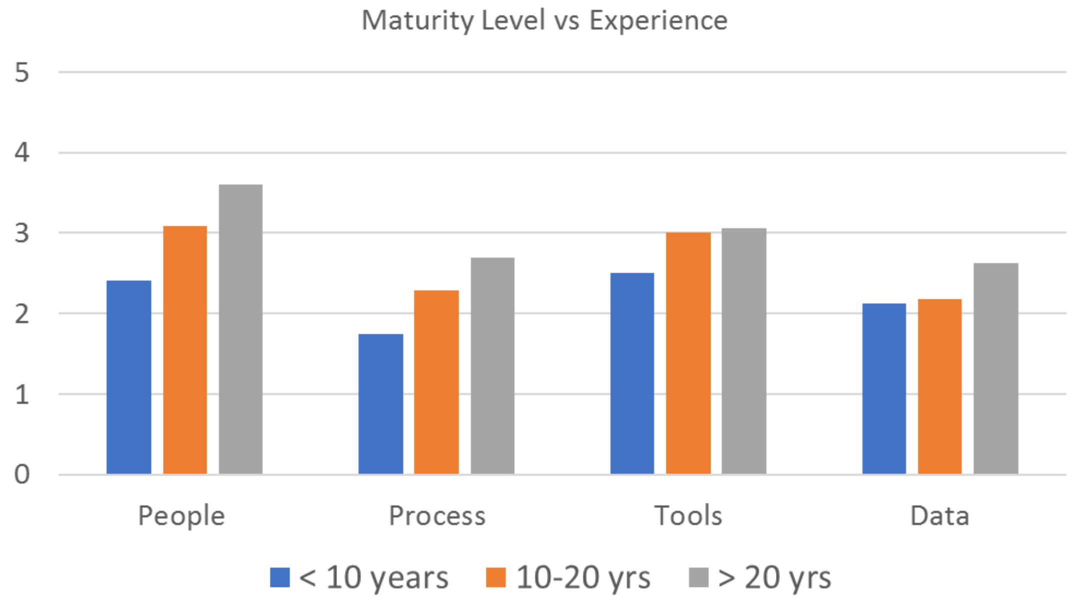

Figure 19: Maturity of the 4 Dimensions vs experience level of the organisation

The result is in line with anecdotal evidence that it takes a long-term sustained effort within companies to reap the benefits from modelling more widely rather than in some individual cases. It also raises the question as to how this process can be accelerated, i.e. how organisations can achieve higher maturity over a reasonable time period, as not many will have investment horizons of 10-20 years.

Considering the variation of maturity across organisations, we obtain the following picture: For the dimension People (Figure 20), there is a pronounced mode at the integrated level, which is reached by 40% of all respondents. The target mode is Level 5, and around 70% aim to reach a Managed or Optimised Level.

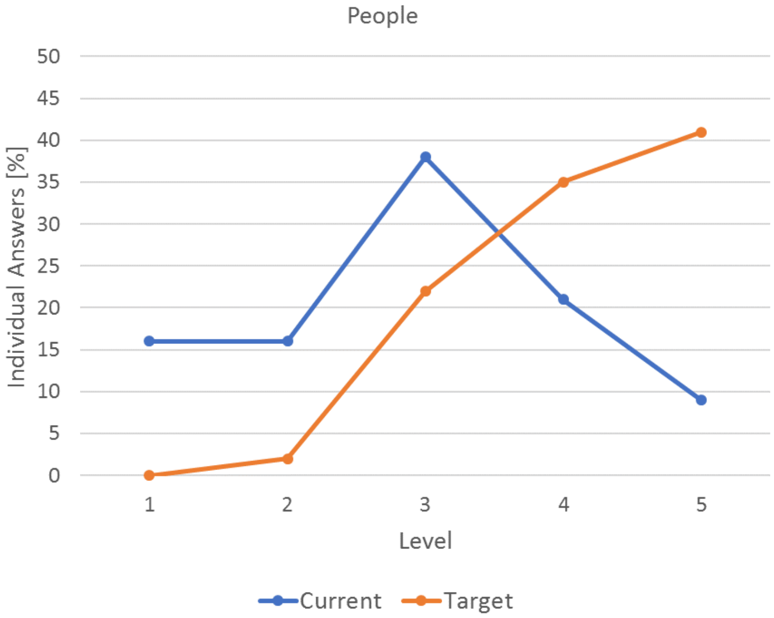

Figure 20: Detailed Results on People. Current (blue ribbon) and target (orange ribbon) maturity: Initial (1), Defined (2), Integrated (3), Managed (4), Optimised (5)

The maturity in Tools (Figure 21) is more diverse than with People; 20% are on the Initial, 25% on the Defined and 30% on the Integrated Level. For over 35% of participants the target was to reach a Managed Level.

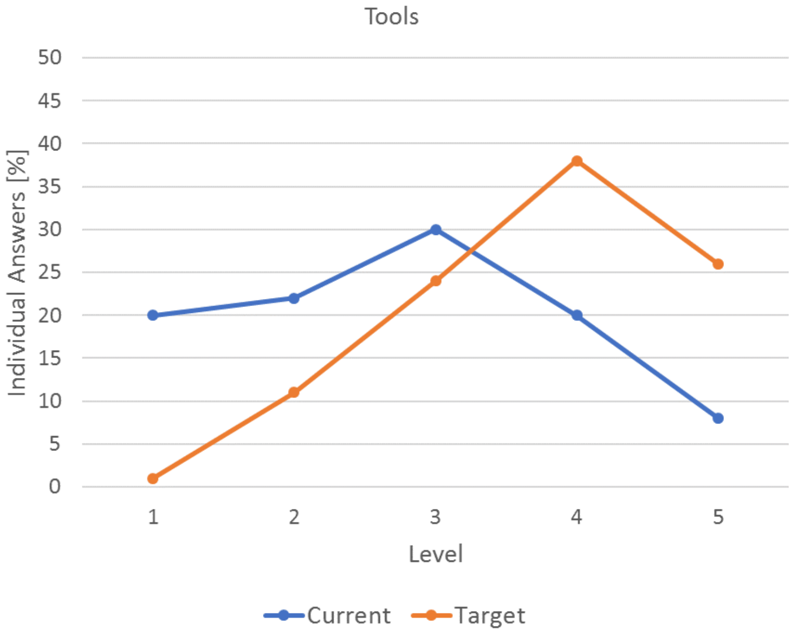

Figure 21: Detailed Results on Tools. Current (blue ribbon) and target (orange ribbon) maturity: Initial (1), Defined (2), Integrated (3), Managed (4), Optimised (5)

The maturity reached in the Process dimension (Figure 22) is for the majority on the Defined and Integrated Levels. Nobody has reached an Optimised Level. For about 30% of participants the target was to reach a Managed Level.

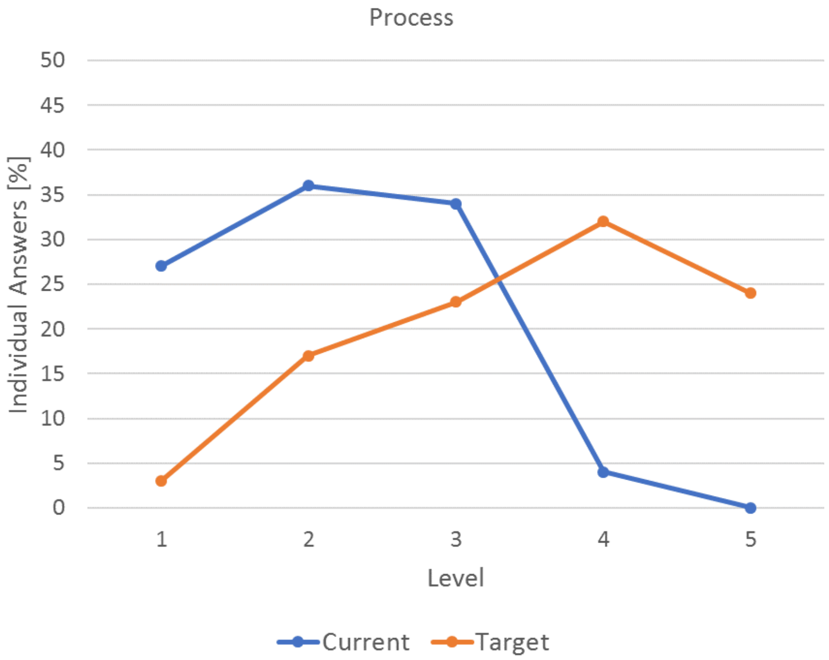

Figure 22: Detailed Results on Process. Current (blue ribbon) and target (orange ribbon) maturity: Initial (1), Defined (2), Integrated (3), Managed (4), Optimised (5)

The maturity reached in the Data dimension (Figure 23) is for the majority on the Defined and Integrated Levels. Similar to Process, almost nobody has reached an Optimised Level. For about 60% of participants the target was to reach a either an Integrated or Managed Level.

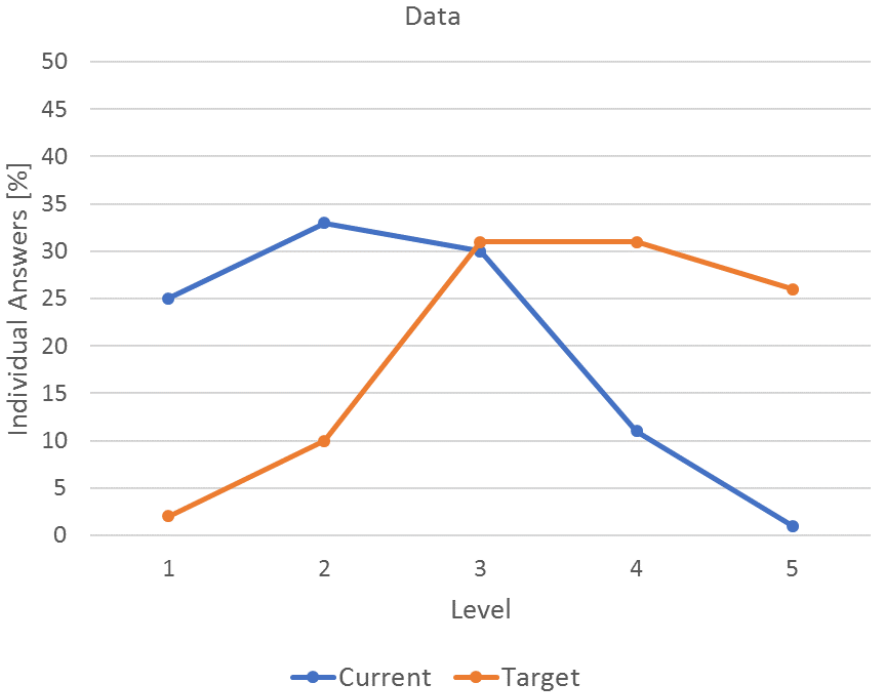

Figure 23: Detailed Results on Data. Current (blue ribbon) and target (orange ribbon) maturity: Initial (1), Defined (2), Integrated (3), Managed (4), Optimised (5)

4.6. Variations within each Dimension

In the following we will analyse the survey results in more detail to understand the current state and target growth in the specific 'pillars' of each of the dimensions.

In the People dimension, the survey asked in detail about the following pillars:

- **Collaborations:** To which extent does your organisation support collaboration on Modelling topics with external partners such as academia, industry, suppliers or customers?
- **Active Recruitment:** To what extent did you actively recruit your materials modeller(s)?
- **CPD:** (Continuous Professional Development) To which extent do you develop your materials modeller?
- **Role Modeller:** To which extent does your organisation define the role of a Materials Modeller?
- **Share Expertise:** To which degree do you share modelling expertise, i.e. to which extent is it accessible to all of the company?
- **Peer Interaction:** To which extent does your modeller interact with their peers?
- **Translation:** How important is the translation of business issues into modelling tasks?
- **Role Modelling:** To what extent does the wider business understand the role of Materials Modelling?

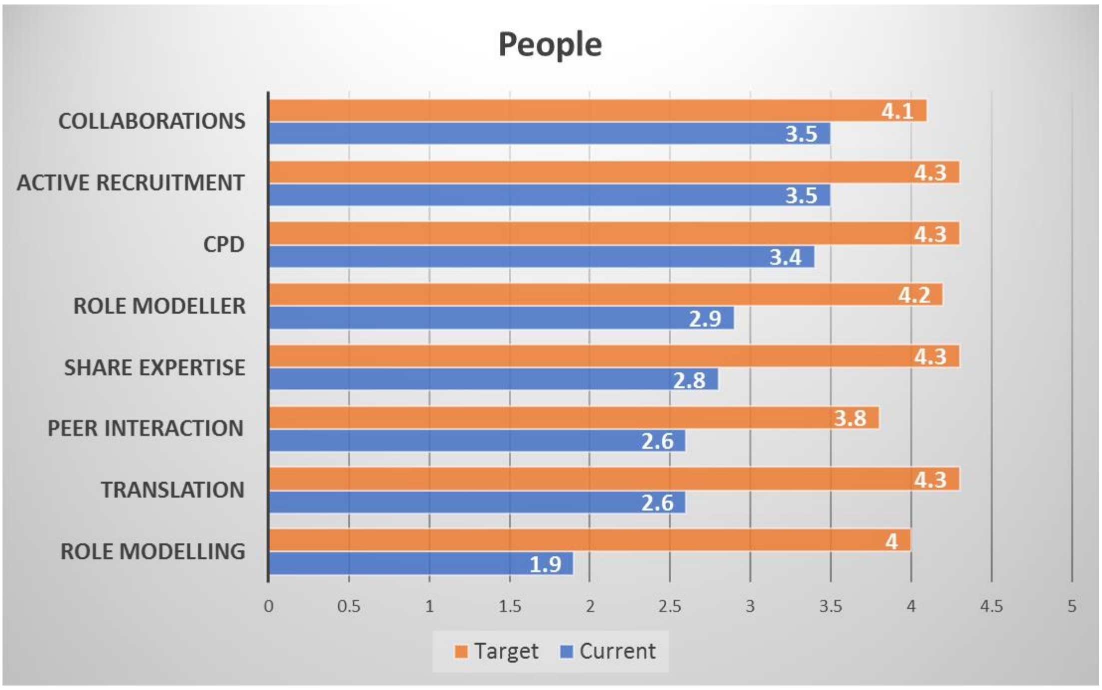

Figure 24: Detailed maturity levels of the People Dimension

As can be seen in **Error! Reference source not found.**, there is a distinct difference in maturity between activities such as collaborations, recruitment and CPD, which have relatively high maturity, possibly because they are often governed on an enterprise level, and the role of modelling, translation and modeller peer interactions which are at a lower level and likely to be less in focus at the enterprise level.

In the Tools dimension, the survey asked in detail about the following pillars:

- **Version:** How important is it for you that your modelling software is on the latest version?
- **Hardware:** What is the status of the hardware you provide for modelling?
- **Applicability:** How would you rate your knowledge of your materials modelling software tools you use and do you know how applicable to your problems they are?
- **Purchase:** How advanced is the process of purchasing your modelling software?
- **Model Maturity:** To which degree can you judge the maturity of the materials models you use, i.e. do you have a good knowledge and control of their accuracy, degree of validation etc.
- **Multiscale:** How advanced are you in the usage of multiscale modelling?
- **Integration:** To what extent is your modelling software well integrated with your other tools (i.e. other modelling tools, LIMS, ELN, enterprise platforms, business decision systems, etc.)?

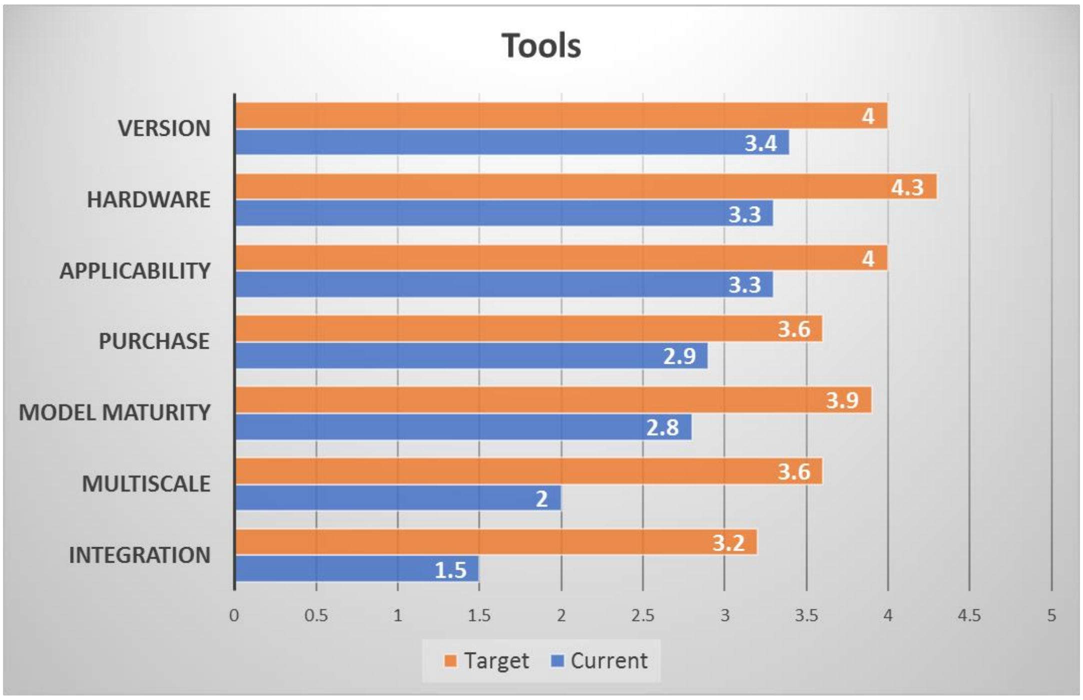

Figure 25: Detailed maturity levels of the Tool Dimension

As can be seen Figure 25, dealing with versioning, hardware, applicability of the software and purchasing as well as model maturity are all roughly at the Integrated level. In contrast, dealing with multiscale modelling and integration of materials modelling with other tools remains a challenge.

In the Process dimension, the survey asked in detail about the following pillars:

- **Mat Mod Impact:** To what extent do you measure the impact of Materials Modelling as a tool to assist in problem-solving, process optimisation, product development?
- **Mat Mod influence:** To what extent does materials modelling influence your decision making?

- **Translation Doc:** To what extent do you document your translation process, i.e. how do you get from a business issue to a modelling activity?
- **Mat Mod featuring:** To which degree does materials modelling feature in your company?
- **Product Life Cycle:** To which degree is materials modelling contributing to the life cycle phases of your products (design, planning, engineering, production, services & recycling)?
- **Improved Product:** To which extent does modelling help you when you analyse customer data to increase customer insight and come up with an improved offer/product?
- **Vertical Chain:** How would you rate the degree of using modelling of your vertical value chain (i.e. mostly internal going from lab-scale to production)?
- **Horizontal Chain:** How would you rate the degree of using modelling in your horizontal value chain (across supplier, distributor, convertor, brand owner, consumer)?

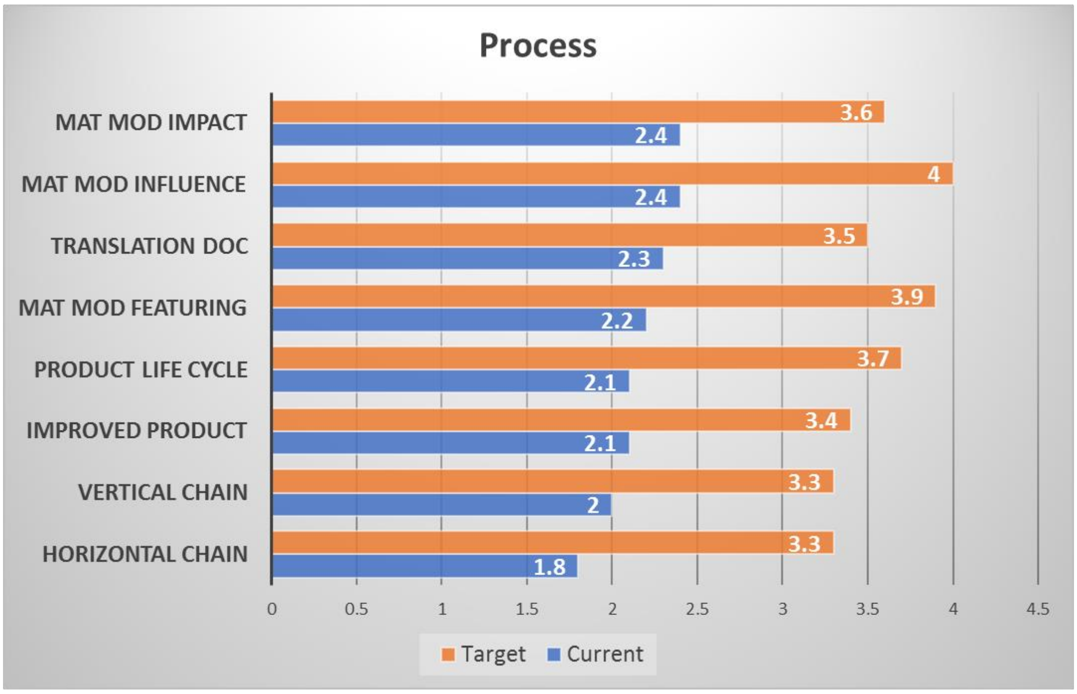

Figure 26: Detailed maturity levels of the Process Dimension

As can be seen in Figure 26, there is not a big variation in maturity levels across the Process pillars, which are mostly between the Defined and Managed levels. Horizontal Value chain interaction is weakest, a pillar which has high growth potential as will be discussed below.

In the Data dimension, the survey asked in detail about the following pillars:

- **Mod + Exp Data:** How important is the usage and analysis of data from modelling together with data from experiments?
- **Analytics Awareness:** How would you rate your modelling data analytics awareness?
- **Data Storage:** How advanced is the level of saving your modelling data?
- **Data Presentation:** How would you rate your capability of presenting materials modelling data within your organisation?
- **Data Sharing:** To what extent do you share your modelling data?
- **Data Awareness** How would you rate your materials modelling data awareness?

- **Mod + Business Data:** How important is the usage and analysis of data from modelling together with business data sources (customer, suppliers, KPIs, finical forecasts, etc.)?

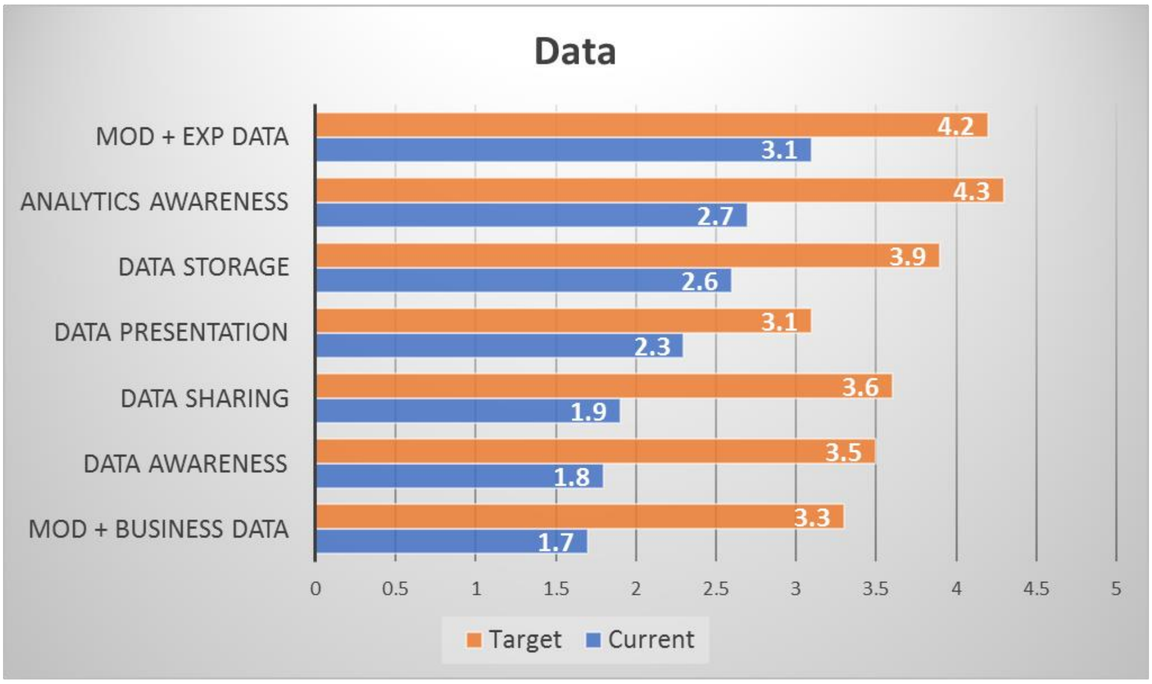

Figure 27: Detailed maturity levels of the Data Dimension

As can be seen in Figure 27, there are considerable differences between the pillars. Integration of modelling and experimental data has become a managed level activity while the low levels of data awareness concerning materials modelling data is quite low, in particular considering the increased attention on data in the context of digitalisation, machine learning and AI. Weakest is the integration with business aspects, which ties in with the relatively low level of translation maturity found in the People and Process dimensions.

5. Change Strategy

As discussed in Chapter 3, careful planning and benefits management is required to ensure these targets are achieved. We will discuss subsequently, what barriers are expected and how change can be managed to overcome them.

To enable the uptake of materials modelling in industry all four dimensions of people, tools, process and data have to be strengthened. For example, the U.S. Department of Defence (DoD, 2018) developed a Digital Engineering strategy in cooperation with stakeholders across government, industry, and academia which led to an identification of 5 goals they have to achieve:

1. Formalize the development, integration, and use of models to inform enterprise and program decision making. (TOOLS)
2. Provide an enduring, authoritative source of truth. (DATA)
3. Incorporate technological innovation to improve the engineering practice. (PROCESS)
4. Establish a supporting infrastructure and environments to perform activities, collaborate, and communicate across stakeholders. (TOOLS, PROCESS)

5. Transform the culture and workforce to adopt and support digital engineering across the lifecycle. (PEOPLE)

We can clearly identify the need of strengthening all four dimensions as a MUST for successful implementation of digital engineering/materials modelling.

To gain further insight and inform industry in decision making, we use the maturity survey responses to perform a gap analysis comparing the “to be” and “as is” maturity levels in each of the pillars of the respective dimensions. Also, responses regarding current barriers pertaining to the different dimensions will be discussed. Potential actions, i.e. Enabling Changes, are described to overcome barriers and address the gaps.

5.1. People

As can be seen in Table 11, the biggest maturity growth is sought for a better shared understanding of the role of materials modelling across the organisation (2.1) followed by stronger translation activities (1.7) and sharing expertise within an organisation (1.5). A higher maturity is also desired for the role a modeller has in an organisation (1.3) and for peer interactions (1.2). Lesser maturity growth is aimed at in CPD (0.9), active recruitment (0.8) and collaborations (0.6).

Table 11: People: Pillars and Maturity Gap

Pillar	Maturity Gap
Role Modelling	2.1
Translation	1.7
Share Expertise	1.5
Role Modeller	1.3
Peer Interaction	1.2
CPD	0.9
Active Recruitment	0.8
Collaborations	0.6

5.1.1. Role of Modelling, Translation and Sharing of Expertise

The role of modelling in an organisation, translation and expertise sharing activities go hand in hand. Emphasizing the translator function helps bridge the gap between modellers and industry stakeholders as translation integrates business KPIs into the use of modelling and communicates business value of materials modelling. This is also a great vehicle to share materials modelling expertise with the wider organisation. Organisations hence need to develop a more differentiated approach to the different roles involving modelling in the organisation.

Furthermore, as the Corning and QuesTek case studies have shown, QBTM is an excellent framework for establishing where modelling can accelerate a value chain and analyse by how much. Similar analysis can greatly contribute to establishing a wider understanding and appreciation of the role of modelling.

5.1.2. Role of the Modeller and better Peer Interaction

The definition of the role of a modeller and establishing better peer interactions can be promoted by clarifying and making decisions on the target benefits of modelling, followed by tracking and continuous improvement as was discussed in Section 3.3. Benefit management in modelling projects

5.1.3. Active Recruitment, CPD and Collaboration

Organisations are aware that clear job specs and an offer of CPD attract valuable workforce. However, respondents shared evidence that there is a lack of differentiation, since “materials modeller” is as wide as a description as “chemist”. Organisations will generally not hire “chemists” but persons specialised in a particular field, such as NMR, formulation, synthesis, etc. It is also up to the individual modeller and organisations such as universities, professional bodies to also bring more clearly recognised sub-disciplines to the profession of “materials modeller”.

Despite the relatively low gap, recruitment and CPD were mentioned by respondents as key barriers in the sense that the materials modelling job typically requires a huge depth of domain knowledge combined with translation/communication skills, hence it is difficult to recruit and train staff. Also, the lack of (continued and sufficiently large) investment was mentioned, i.e. that often there are too few modellers to make a real difference. This also ties in with the long-time increase of maturity, especially in the People dimension.

5.2. Tools

As can be seen Table 12, the biggest maturity growth is wanted for the better integration (1.7) and multiscale modelling (1.6). A higher maturity is also wanted for the maturity of models used (1.1) and better hardware access (1.0). Lesser maturity growth is wanted in the purchase process around the software (0.7), knowledge about software applicability (0.7) and having the latest software version (0.6).

Table 12: Tools: Pillars and Maturity Gap

Pillar	Maturity Gap
Integration	1.7
Multiscale	1.6
Model Maturity	1.1
Hardware	1
Purchase	0.7
Applicability	0.7
Version	0.6

5.2.1. Integration and Multiscale Modelling

There is a big appetite in industry to have better integrated models and thereby enable multi-scale and/or multi-physics modelling. Such maturity growth cannot be achieved without a collaborative effort between all stakeholders, in particular software users (SWUs) and software owners (SWOs) to reach wide agreement on interoperability standards as a basis for SWOs to provide industry-ready integrated, standardised, interoperable software solutions. The EMMC has been active in this field, leading to the recent release of the European Materials & Modelling Ontology (EMMO) (Friis, et al., 2019).

Hence, manufacturing industry only has limited control over advancing maturity in the areas of integration and multiscale modelling. Strong collaboration and further technical advancements are very much needed.

5.2.2. Maturity of Models

As in the case of multiscale modelling, advancing the maturity of models depends on a range of actors. Respondents consider for example the lack of knowledge of accuracy and lack of validation as key barriers. Only a well verified and validated model can deliver a reliable ROI, hence industry is also called upon to collaborate and invest more in this area, for example by agreeing on "benchmark" validation tests similar to those widely used in engineering simulations.[7]

5.2.3. Hardware

Hardware is generally not a problem for organisations with a high modelling maturity. Modelling was established at least three decades ago and one could gradually increase hardware synchronised with recent code developments (HPC, GPUs, etc.). Organisations that have started modelling more recently and SMEs may struggle with deploying hardware. Hardware requires its own ecosystem of people, tools, process and data, which is very costly to establish from scratch. Thus, one can consider to put a 3rd party in charge of their maturity and look into SaaS or Cloud services.

5.2.4. Software: Purchase, Applicability, Version

Purchase procedures and access to the latest version of software are typically well managed in industry. Also, the industrial SWUs are very aware of what their tools can do. However, internal wiki style webpages can help to share also with non-experts what problems can be solved with which tool.

5.3. Process

As can be seen in Table 13, the biggest maturity growth (in the range of 1.5-1.7) is sought for the featuring and influencing of materials modelling in decision processes and that it plays a role in the product's life cycle and horizontal value chain. A lesser maturity growth (1.3) is sought for modelling featuring in the vertical value chain and improving products with customer data. There is also a need for better translation documentation and measuring the impact materials modelling has on a project (1.2). The Process dimension needs to grow more than one maturity level in all aspects to satisfy the wished-for targets.

Table 13: Process: Pillars and Maturity Gap

Pillar	Maturity Gap
Mat Mod featuring	1.7
Product Life Cycle	1.6
Mat Mod influence	1.6
Horizontal Chain	1.5
Vertical Chain	1.3
Improved Product	1.3
Translation Doc	1.2
Mat Mod Impact	1.2

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[7] https://www.nafems.org/publications/benchmark/

5.3.1. Impact of materials modelling and influencing decision processes

Using the Business Processes analysis and 4D-QBTM provides the modelling function in industry a framework for demonstrate where and how materials modelling creates an impact modelling on an existing business process. KPIs for improved efficiency and effectiveness can be highlighted and tracked in this framework.

Current key barriers according to input received from modellers are a fragmentation of processes and that digital continuity is in its infancy. Also, there is a lack of standards which prevents integration of models into R&D workflow for the most impact.

5.3.2. Impact on product life cycle and the horizontal value chain

The perspective on the life cycle of a product has been moving towards “cradle to cradle” and circular economy[8]. Making this vision a reality will require deep knowledge about all aspects of a product, including the detailed chemistry of materials in a product, see also (BOEING, 2015). Models and digital representations will play an increasing role.

Likewise, materials models are becoming more important in the horizontal value chain across supplier, distributor, convertor, brand owner, consumer, both as a means of exchanging information and as an add-on to a product, a concept sometimes referred to as Product +. Examples include materials relations tuned to the specific materials produced that support manufacturers in the simulation of materials processing[9]. Modelling can also aid with answering “what-if” questions due to suppliers offering different starting materials and customers demanding different ingredients.

5.3.3. The vertical value chain and improving products with customer data

The vertical value chain goes from lab-scale to production and this is naturally where modelling can aid. What is needed to reach a higher maturity are better reporting processes. There needs to be a process that captures the benefits, efficiency and effectiveness. This gives visibility to materials modelling in the organisation and also quantitative evidence why modelling should be used in the vertical chain. Improving products with customer data will happen more and more in the near future as customers are becoming more critical about ingredients.

5.3.4. Documentation of Translation

A good translation document should evidence good understanding of the business case and the manufacturing processes. It should make an inventory of people, tools, processes and data available and then suggest which modelling workflows are accessible. The document should propose actors (i.e. people) who would do the modelling and propose strategies to validate the chosen models. Finally, it should comprise an end report that translates the modelling results into information usable by the organisation. Useful material that can help an organisation achieve a better maturity was published by the EMMC (Hristova-Bogaerds, et al., 2019).

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[8] https://ec.europa.eu/regional_policy/en/newsroom/news/2016/01/28-01-2016-real-economy-cradle-to-cradle-powering-europe-s-circular-economy

[9] See e.g. http://www.performance-materials.basf.us/ultrasim

5.4. Data

As can be seen in Table 14, the biggest maturity growth (1.7) is wanted for data sharing and awareness. This is followed closely by better data analytics and combining business and modelling data (1.6). A growth in maturity of at least one level is wanted for data storage (1.3) and combination of modelling with experimental data (1.1).

Table 14: Data: Pillars and Maturity Gap

Pillar	Maturity Gap
Data Sharing	1.7
Data Awareness	1.7
Mod + Business Data	1.6
Analytics Awareness	1.6
Data Storage	1.3
Mod + Exp Data	1.1
Data Presentation	0.8

Many of the companies we interviewed are undergoing a digitalisation process, hence there will be a foreseeable improvement in the data maturity. Materials modelling can use this as a vehicle to become even more useful. If large, consistent data spaces are expected, machine learning/materials modelling combinations will become an asset.

5.4.1. Data sharing and Data awareness

Respondents noted a lack of sharing of data thus it will be important to consolidate data into a single consistent searchable format, as well as structuring, storing, and using materials data to harness the power of artificial intelligence. Sharable data need to be FAIR (Wilkinson & al., 2016), i.e. Findable, Accessible, Interoperable and Reusable. According to a report by PwC, the cost to the European economy of not having FAIR data is at least €10.2bn every year with a substantial impact on manufacturing industry. A number of initiatives are under way to address the issue, see e.g. https://www.fairsfair.eu/.

5.4.2. Data analytics awareness and the combination of business and modelling data

Useful data analytics can only happen on a large scale when data are integrated with information systems, which is currently lacking. Data analytics requires well curated data, as discussed below. An issue voiced by materials modellers is that data analytics gets added to their tasks, while it requires proper training and resource to complement materials modelling.

The combination of business and modelling data is in its infancy; however, closer alignment of modelling activities with a companies' business processes, as has been discussed in the White Paper, will go towards addressing this gap. Business Decision Support Systems are Enablers and their integration with materials modelling integration of materials modelling (Belouettar, et al., 2018) the Enabling Changes contributing to closer alignment.

5.4.3. Data Storage

The actual physical storage is not a problem rather the fashion in which data are stored. A data management plan (DMP) is key and one has to assess whether the investment to store the data balances the return on investment that the reuse of the data can give. The EMMC provides a DMP template[10] which can be adapted to an institute's policies and recommendations. A good source of information is FAIRsharing[11], a community-driven resource.

5.4.4. Combination of modelling and experimental data and presentation of data

The combination of modelling and experimental data happens regularly to validate models and as parameters in data-based models, which have a long tradition in the chemistry and materials modelling field as "Quantitative Structure Activity/Property Relations (QSAR/QSPR). What is still in the fledgling stages is the usage of experimental data to build new materials relations. All respondents felt very comfortable with presenting data to their peers would like to see more opportunities to present to stakeholders higher in the business hierarchy.

6. Investment strategy

A survey conducted in 2016 on information provided by 29 companies (Goldbeck & Court, 2016) covering a wide range of sizes and industry sectors and an even distribution in terms of types and scales of modelling revealed the willingness of industry to invest in materials modelling. The total materials modelling investment (covering staff, software and hardware) ranged from €45K to €4M (average €1M, median €0.5M). Staff was the largest cost factor whereas investments in software were five times less and investments in hardware 16 times less, respectively. However, cost savings due to involving materials modelling in projects ranged from €100K to €50M (average €12M, median €5M). The ROI, determined by the ratio of revenue generated and investment in modelling, ranged from 2 to 1000. Removing the largest and the smallest values yields an average ROI of 8. A trend for ROI to grow more than linearly with investment in modelling was found.

In making investment decisions for example across hardware and software, organisations need to consider whether materials modelling, or at least the models that are used and generated is an expense or an asset (Hanson, 2010). Materials Modelling activities would fall under R&D activities and suffer from the fact that it is not a priori clear what the right size of an investment should be as there is not simple way to quantify R&D. Under Generally Accepted Accounting Principles (GAAP) firms are required to expense R&D in the year spent (Valens Research, 2016). However, capitalising R&D costs (see Chapter 2.2.2) shows them as an asset on the balance sheet of a company. Materials modelling per se (including associated data, validation and know-how) should undergo 4D-QBTM to recognise the true value of investing in it.

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[10] https://emmc.info/emmc-info-data-management-plan-template-dataset-description/ kindly provided by the collaboration of the European Funding Division of Warrant Group Srl, within PARTIAL-PGMs project GA n. 686086.

[11] https://fairsharing.org/

7. Conclusions

The strategies for industry to engage in materials modelling and to build up a successful and impactful materials modelling capability can be summarised as follows:

1. Perform an assessment of the dimensions people, tools, process and data in your organisation using the EMMC Materials Modelling Maturity Model. Identify the *status quo*.
2. Perform a 4D-QBTM on your business process and identify which specific Enablers (i.e. pillars of the dimensions people, tools, process and data) can support your targeted business benefits. Specify relevant effectivity and effectiveness metrics.
3. Use benefit analysis and play through what-if scenarios: if you had additional/different people, tools, processes or data, could you get more benefits? Are these valuable to your organisation? Build a benefits dependency network to determine Enabling changes.
4. Revisit the Maturity model and look into the pillars of each dimension and see which ones (i.e. specific Enablers) you need to mature and how, in order to bring about the desired changes.
5. Apply new strategy and provide 4D-QBTM and full metrics to evidence success.

8. Acknowledgements

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9. Glossary of Terms and Abbreviations

AI – Artificial Intelligence

AIChE - American Institute of Chemical Engineers

API – Active Pharmaceutical Ingredient

BDSS – Business Decision Support System

CADD – Computer Aided Drug Design

CEN - Comité Européen de Normalisation (English: European Committee for Standardization)

CMMI - Capability Maturity Model Integration

CPD – Continuous Professional Development

CWA – CEN Workshop Agreement

DMP – Data Management Plan

DoD – U.S. Department of Defence

EMMC – European Materials Modelling Council

FTE – Full Time Employee

ICME - Integrated Computational Materials Engineering

IDC - International Data Corporation

IRR - Internal Rate of Return

KPI – Key Performance Indicator

MGI – Materials Genome Initiative

ML – Machine Learning

MODA – Modelling Data

N/A - common abbreviation in tables and lists for the phrase “not applicable”, or “not available”.

NASA - National Aeronautics and Space Administration

NIST - National Institute of Standards and Technology

NPV – Net Present Value

QBTM – Quantitative Benchmark of Time to Market

ROI – Return on Investment

SWO – Software Owner

SWU – Software User

TCO - Total Cost of Ownership

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