Translation in Materials Modelling – Process and Progress

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1. Executive Summary

The EMMC[1] Translators Guide (Hristova-Bogaerds, et al., 2019) provides a vision for industrial users (Clients) how to benefit from a systematic materials modelling translation process, that covers translating an industrial need/challenge into a solution by means of materials modelling and simulation tools. The experts that are performing this process of providing a Translation service are called Translators in Materials Modelling. They often act as a team and propose an assistance and consulting for companies. Translator(s) can be either academics, software owners, independent consultants, modellers or code developers with the relevant expertise, and even be employees of the Client company.

The EMMC Translation concept for materials modelling was collaboratively developed by engaged European Stakeholders from industry and academia in a bottom-up approach facilitated by the European Union and the EMMC within the EMMC-CSA project[2]. The aim of the Translators Guide (Hristova-Bogaerds, et al., 2019) is providing Translators with an (orientation) basis which they may follow in an agile and personalised way, to facilitate and safeguard a successful and efficient mutually agreed workflow (course of action) in an industrially oriented modelling project.

In the current contribution, we aim to further contextualise the Translators Guide with Translation scenarios that have evolved since the EMMC-CSA project ended in 2019. The interdisciplinary team of authors will give an outlook focussing on tools under development, opportunities upon maturing (learning by doing) and challenges from diversification that we expect to manifest in the 2020s. We aspire to provide some updating and enriching of the previous EMMC findings for this multidimensional, multidisciplinary and highly communicative pillar of materials modelling. We aim to make the proposed six translation steps more transparent. Stakeholders shall find suitable and applicable starting points which they can use as base towards adaption of their organisations' internal standards and processes. Still, we are convinced that a trustful and harmonised proceeding performed by stakeholders of different domains will be an active catalyst for boosting material innovation by:

- … simplifying joint projects among regional SMEs or multinational large-scale industry
- … involving end users and application perspectives in a holistic view
- … facilitating the implementation of overarching aims such as sustainable and economically attractive materials development.

The central idea is explicating an effective and efficient Translation process by sharing the experience of the authors and facilitate and support both the Client and the Translator. They are guided to follow, apply and subsequently, perform PDCA (Plan, Do, Check, Act) approaches[3] which are needed to evolve the Translator Role and process for future ventures such as OntoTrans[4]. Performing a conjoint Translation process, thus, is a catalyst for impactful Materials Modelling.

[1] European Materials Modelling Council, www.emmc.eu
[2] EMMC-CSA H2020 project, Grant Agreement No 723867
[3] www.iso.org/tc176/sc02/public
[4] https://cordis.europa.eu/project/id/862136, www.ontotrans.eu

2. EMMC Translation – A Retrospective

In February of 2014, a workshop[5] brought interested parties together to discuss and report on the state of the art in the materials modelling field by identifying the most promising areas for future research and innovation. There was, notably, a gap in awareness, knowledge and skills that hampered industry to unlock the potential benefit of current modelling technology. In manufacturing companies, modelling was typically found within the realms of R&D and industrial scientists were not always focussed at translating and communicating in joint projects with business units. Manufacturing "end-users", in particular SMEs, quite often had a lack of expertise that prevented them from integrating materials modelling into their development and production workflows. The workshop participants established that there was a need for new players who have the ability to "translate" industrial problems into project-specific cases to be simulated. From this point in time, these new players were referred to as "Translators" and their role was assigned to close the "language gap" between industrial stakeholders and materials modellers by "analysis of industrial problems and translation into materials modelling cases that can be simulated" (de Baas A. F., 2014). The primary stakeholder within industry interested in profiting from modelling is usually the R&D unit, but the industrial problem is usually set by managers dealing with holistic corporate decisions. Thus, the Translator will have to understand and distinguish how a modelling solution can benefit the business side as well.

Later in 2014, within the Materials Modelling Leadership Council (Ball, Goldbeck, & de Baas, 2014), a team called the Translators Group, had been formed with the mission to identify ways and supporting instruments of how to bridge the "innovation valley of death" starting from the side of the industrial innovation hill by using materials modelling and simulation to materialise sustainable solutions. At the time, Peter Klein took the role as Operational team manager.

From September 2016 to August 2019, The EMMC was funded by the European Union as Coordination through the Coordination and Support Action (CSA)[2], where Translation had its own dedicated work package.

During the EMMC-CSA project, a Translators Guide (Hristova-Bogaerds, et al., 2019)[6] was composed. It is a seminal document describing general principles of Translation work, and establishing an overview in the Translation tasks and required skills. The aim of the Guide is to provide to the modelling community and industry the understanding of the Translation role as well as the industrial needs in the effective Translation. The objective is to reach optimal support in building awareness and confidence in applying materials modelling for a broader adoption, in particular by small and medium-sized enterprises (SMEs). The document can be used not only by Translators but also by (industrial) modellers to discover what to expect from Translators and from the process itself.

[5] Meeting on "EU Policy on modelling, simulation and design", held on February 27th, 2014 in Brussels.
[6] The guide was published online 2017, but emerged in the Zenodo Repository in 2019.

The Guide introduces six generic Translation steps, which indicate how the Translation proceeds and benefits the Client. (Figure 1) (Hristova-Bogaerds, et al., 2019)

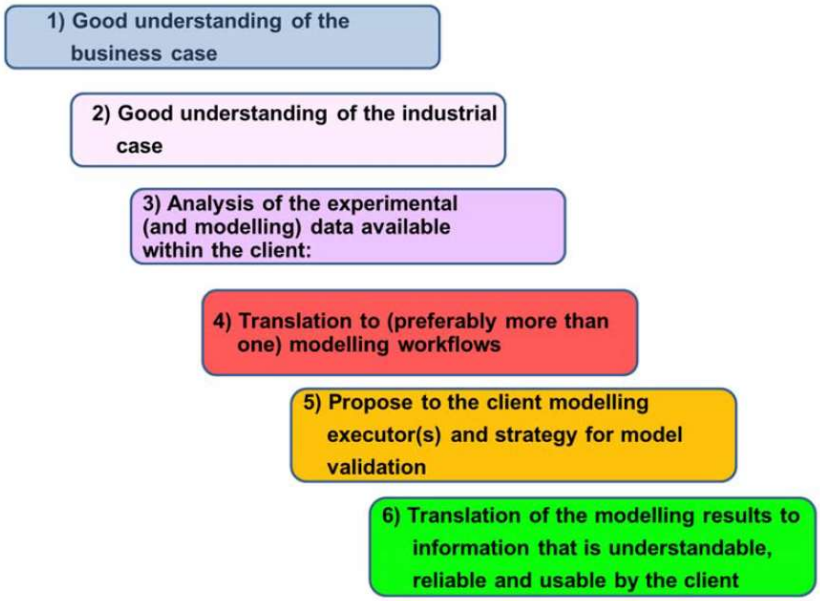

Figure 1. The six universal steps of the Translation process in materials modelling

In the following part of this paper, we will discuss each of these steps and the processes around them and add more insight.

In the course of the EMMC-CSA project, some focused Translation workshops and trainings were provided in the period from 2016 to 2019. Key topics, like the role of Translation, industrial requirements for Translators, benefits of employing a Translator, and training requirements for Translators were addressed and discussed involving a wide range of European stakeholders including manufacturing industries (both SMEs[7] and LEs[8]), software owners and models developers based in academia. The contributions from experienced Translators were significant for the development of Translation methodology and concepts, and subsequently integrated into the Translator Guide (Hristova-Bogaerds, et al., 2019).

The initial Translation expert meeting took place in Eindhoven (NL) in June 2017. The main discussion points were Translation as a role and the fundamental Translation needs of SMEs and LEs. Thereafter, a survey was initiated to gather information and deduct from it how the community envisages the Translation process. The results of the survey were then discussed at the EMMC Translation Workshop on September 2017 in Brussels (BE), which was co-hosted by the European Commission. The outcome led to the definition of the six steps of Translation with the intention to provide fundamental guidelines. Industrial views and needs for Translation were considered in the frame of a focused workshop in December 2018 in Eindhoven (NL). Education for Translators and requirements for Translation training were the topics of a second expert meeting in Hamburg (DE) in March 2019.

Additionally, two sessions at both the EMMC International Workshop in 2017 and 2019 in Vienna, (A), respectively, and a session at the EMMC Workshop on Industrial impact of materials modelling in Turin (IT) in July 2019 had a focus on Translation and Training for companies related topics. Many of this

[7] Small and Medium-sized Enterprises
[8] Large Enterprises

papers' authors and persons involved with Translation took the findings from 2019 and are evolving them further in their professional careers and are adding new experience. Thus, Translation is very much contemporary and active as shown by the Mini-Symposium at the 14th WCCM & ECCOMAS Congress (Konchakova & Klein, 2021) and also a tutorial workshop which was organised during this event.

During the course of the EMMC-CSA project, 17 case studies (Pezzotta, et al., 2021) using the EMMC Translation case template (see Appendix 1) and the EMMC Translators Guide, were collected.

The major outcomes and the consensus from all of these meetings and discussions can be summarised in the following conclusions:

- Performing Translation in materials modelling is a role, which can be adopted by individuals or, more likely, by a **team of Translators**. A team comprises professionals who can estimate the modelling efforts, advice the Client in the solution approach and forecast results (both business and modelling related aspects) of the industrial related project. Thus, it is an interdisciplinary team of experts with skills required to perform the Translation process. In some cases, these teams can include experts from the Client's institution, as especially LEs have means of a computational infrastructure and modelling expertise. Moreover, they have modelling specialists, who may play already the role of Translators. At the same time, SMEs have lack of modelling specialists, expertise and infrastructure. That is why **Translation for SMEs** requires more efforts and guidance than Translation for large companies.
- Depending on the modelling project focus and specifics a certain workflow will have to be established, and this led to the six **Translation steps** which will be discussed in detail below. It should be noted that the order of the steps could be varied depending on the Client preferences, focus or stage of the project, and open issues. Moreover, sometimes Translator could not be involved in all of six steps of the Translation process.
- A formation of a concise and reliable **Translators' database** would be beneficial for SMEs. It could be relevant to vet these professionals via a rating system and/or the provision of successful Translation cases as a reference.
- Translation is an **iterative process**. Translators should be in touch with the Client and discuss the evolution of the project regularly for an efficient and successful Translation.
- **Timelines** in academia are still very different from timelines in industry. Often industrial problems cannot wait for months or years to be solved. This requires quick action, transparent scheduling and flexibility from the Translation Team.
- Translation could be provided by employees of the Client company. In this case, we are referring to **internal Translators**. They are employed by the Client and support directly the business interest of their organisations.
- If a Client (SMEs or LEs) employs an external modelling specialist to execute the Translation and provide modelling support of an industrially relevant simulation, we are referring to **external Translators**. They are independent Translators (usually from Research Institutions, consulting firms or Software companies), who are working on project-to-project basis with manufacturing industry and provide Translation as a service.
- Translators need to understand the corresponding **techno-economic impact** for the customer (SMEs and LEs) and provide a statement of work (SOW) that clarifies the deliverables, gives an estimation of schedule, costs and benefits, analyses ROIs, and ideally links modelling activity to business impact.

- **Neutrality** is the most discussed and difficult term to agree on. Neutrality is expressed by placing the specific interest of the Client always before the transparent interest of the Translator. Translators can be part of the modelling execution if this is of benefit of the Client. Translators need to provide the Client with more than one modelling solution, and propose models and modelling strategies that offer the best solution within the framework of the industrial problem. If the translators propose their own preferred models, they need to give a good justification why they may be the only/most suitable models for the problem of the industrial Client. The industry should expect this from the Translator or even ask for it.
- Translators should advice the end-user/Client in the decision-making based on the modelling results using business relevant data. Often it is necessary to ask and operate with proprietary information. **Confidentiality** and **trust** between Translator and Client are very significant aspects and should play a key role in the Translation practice, framed by clear-cut agreements.
- To convince new Clients, Translators will need to provide some evidence which can demonstrate their professional integrity. Translation documentation could be prepared in the form of **Translation cases** using the EMMC template (see Annex 1 of this paper). If permitted by a Client, publication of the workflows of these Translation cases in open repositories could be extremely beneficial for both Translators and industrial end-users.
- Translators should **understand different models** and what they can be deployed for. Besides knowledge of predictive (physics-based) models a good understanding of data-driven models based on machine learning or Artificial Intelligence (A.I.) becomes more and more important/applicable.
- **Continuous professional development** is a key: Translators need to obtain and sustain both modelling and economic related knowledge. In particular, education on basic economic impact analysis is highly recommended. Soft skills, training regarding software capability, licensing scenarios and Intellectual Property (IP) are key knowledge for all types of Translation. Translators need basic skills to evaluate the return versus investment and accuracy of their proposed modelling flows. The information needed for this analysis should be provided by the modellers: accuracy, validation, benchmarking in generic conditions of the models, simulation time, and computer power). Also, software owners can be helpful by providing case studies (usually found in their manual or on their websites), model validation and verification, licences types and fees. Additionally, Translators need to train their communication skills and be an excellent networker and stakeholder manager. Understanding the challenge expressed by the Client within a domain is a key and may require interacting and interdisciplinary Translator teams. Training for Translators could include short **secondments and internships** at industrial end-users to gain detailed understanding of the business and industrial case and to seek confidence with the Client.
- **Certification** of Translators is still an open question, which initiated many discussions, and yet remains unresolved. Currently there is no accreditation or internationally recognised career path for Translators and no official body to certify them. If the Materials Modelling community recognises the Translator role vital, a similar path as taken by Research Software Engineers may be trod.[9]
- A **Maturity Model analysis** (Goldbeck & Simperler, 2019) considered Translation and its current level of maturity at 2.6 on a scale ranging from 1 to 5. The targeted level for Translation is set as 4.3 which shows that industry has high interest to deploy it.

[9] https://society-rse.org/

- **Business models** for Translation providers are currently under development. Some Test-Bed and other projects funded by H2020[10] (for example, OntoTrans[4], OntoCommons[11], MarketPlace[12], VIMMP[13], and VIPCOAT[14]), where Translation plays an important role, are working to evolve the role and a business model around.

3. The Six Steps of Translation

Before we embark into an in-depth discussion of the six steps, we want to revisit certain concepts that will be expedient. As we explained shortly in the previous parts, when we refer to "Translation" in Materials Modelling we mean its definition according to the EMMC, where Translation is the process of translating industrial problems into questions to be solved using a modelling approach, and applied to simulation tools for, e.g., creating industrial innovation. In projects assessing innovation challenges, Translators pick up industrial challenges, transform the (technical) problem into modelling workflows, and guide manufacturers in the execution of computations respectively assist with interpretation and utilisation of modelling results, as depicted in Figure 2.

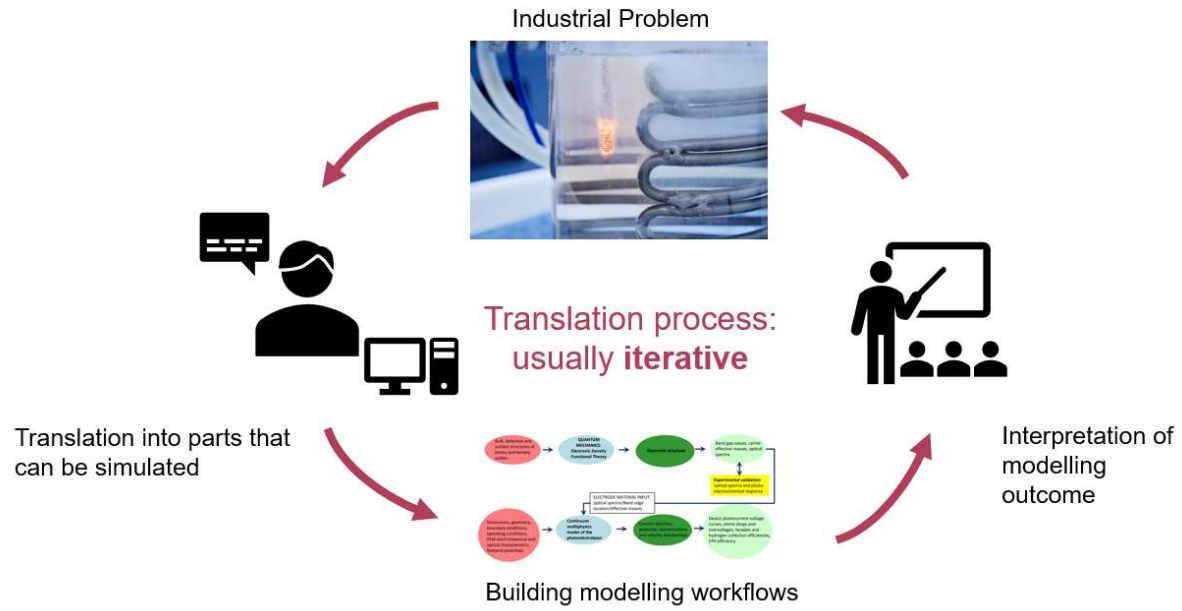

Figure 2. Overview of the Translation process

The process is iterative and can involve both individuals or a team of Translators. The Translators fulfil their industry-project related tasks in interaction with both, an industry Client who requires material data or process related data profiting from materials modelling solutions, and modellers who execute modelling workflows in an effective and efficient way. Modellers can be located in industry or in academia/ software owners/ independent modelling consulting. Ideally, persons operating as

[10] Horizon 2020 is an EU Research and Innovation programme, that was running from 2014 to 2020.
[11] https://cordis.europa.eu/project/id/958371, https://www.ontocommons.eu/
[12] https://cordis.europa.eu/project/id/760173, https://www.the-marketplace-project.eu/
[13] https://cordis.europa.eu/project/id/760907, https://www.vimmp.eu/
[14] https://cordis.europa.eu/project/id/952903

Translators will not be focused on undertaking the various modelling steps but rather on playing the role of a path-breaking guide and facilitator.

Industry often may not be aware of the full potential of modelling and/or may need guidelines in selecting the suitable modelling workflows for solving their problems efficiently and effectively. The modellers may not be aware of the extent of problems in industry that could benefit from joining their skills. The software tools offered may range from codes to be operated from the command line of a Linux machine to commercial software with graphical user interfaces.

The Translator comes in as a professional specialist/expert (or team of professionals) who fulfils a role to understand both worlds – an identified industrial challenge and a wide field of feasible modelling approaches - and speaks "several languages" with "Modelling" being their business fluent mother tongue.

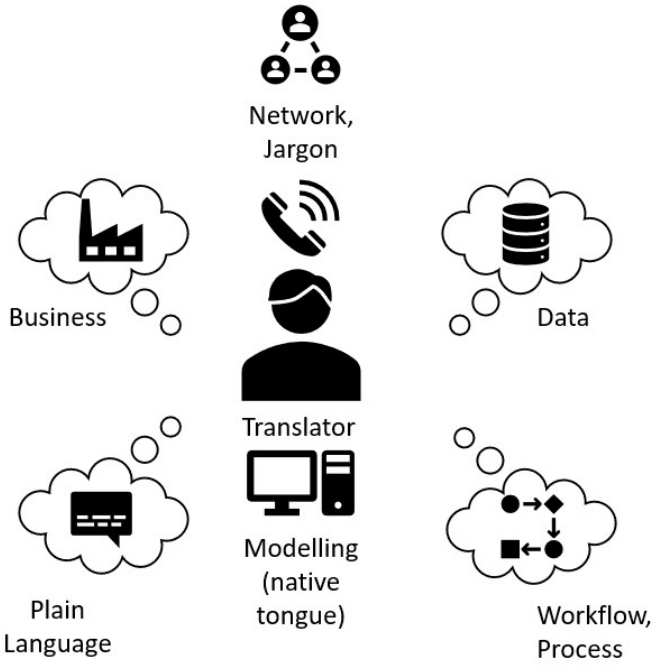

Figure 3. The translator, a "domain-polyglot" and networker

Figure 3 depicts the many "languages" a Translator has to command. If we borrow a concept from linguistic translation (Mraček, 2018), the translation from a language to the translator's mother tongue is referred to as direct translation, while the translation from their mother tongue to any other language is referred to as inverse translation, which is seen by linguists as the more challenging direction. In our case, the "Translation to modelling" can be referred to as direct while the "Translation from modelling" is the inverse Translation. The Translators will have to employ both as they make their way along the six translation steps. They also require a good rapport with their modelling network to find modellers and information.

The Translator Guide (Hristova-Bogaerds, et al., 2019) suggests, besides the aforementioned profound "linguistic skills" the following attributes as beneficial for a Translator in materials modelling complying with the requirements accompanying the translation process:

- **Industrial** background
- Knowledge of economic impact, **KPI**s, **Benefit Management**
- Broad knowledge of **modelling methods** which are commonly used in their field of expertise
- Broad understanding of different experimental **techniques** and data analysis
- **Analytical** skills and aptitude for **problem solving**
- **Communication** skills, needs to listen (Soft Skills)
- Project management skills
- Being neutral – **not favouring** preferred solutions
- Expected to show a proven "**track record**" of expertise on Translation
- Managing **data confidentially**

Certainly, a Translator persona cannot offer all answers to all questions industry may have; hence, we expect experts in particular fields (e.g., steel, alloys, aerospace, medicinal devices, catalysts, etc.) to emerge. These subject experts, however, should have an extensive knowledge of the market, newest developments and upcoming regulatory aspects in their fields; in short, a substantial understanding of where their field is moving to in the future. Therefore, communication skills are required also with respect to communication among translation experts with complementing expertise in a team fulfilling the Translator role.

We recommend to Translators to consider all relevant steps; however, on some they may tread lightly while others may require a firmer step, depending on their assignment and on the project focus.

3.1. Step 1: Good understanding of the business case

In the first step, the Translator aims to consider and understand the business case framing a modelling activity (Figure 4). The Translator will be brought in as a service provider attending to "the business" that constitutes a relation of an industry organisation to its environment, primarily its customers but also providers and end-users. Translators should expect a first meeting with their business Client to be very formal – posing the business case reveals step by step what the company is working on. Before the Client will talk about the business case a non-disclosure agreement (NDA) may have to be signed. Hence, the company will want to protect their ideas and innovations to come and make sure that their objectives in a project that they pursue are lit and illustrated.

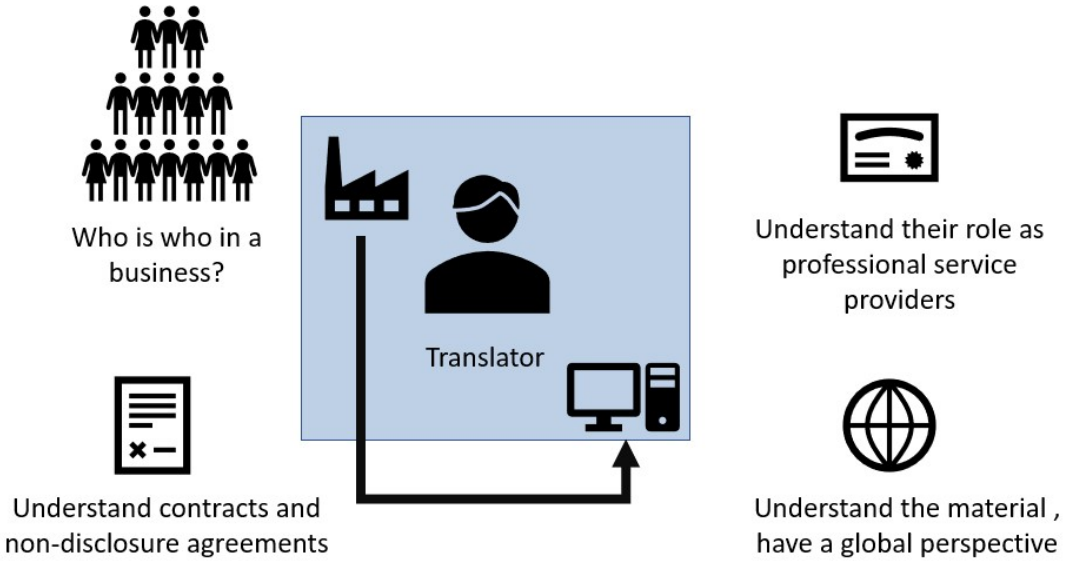

Figure 4. The Translator and the Business, Translation from "Business" to "Modelling"

Once a contract in any form is signed the Translators become liable for their work and their translation efforts will go beyond "helping out a friend from industry". They take responsibility for their service provision and they are liable to terms and conditions as stated in a contract. If the Clients are not satisfied with a provided service, they have the right to stop the cooperation or even take legal steps. Translators working for a company are insured by their employer whereas self-employed Translators may want to invest in private and public indemnity insurance. Sometimes, Clients may ask if the Translators can provide these. The contract should also state who owns intellectual property rights should key exploitable results emerge.

Translators need to understand the work laws on a national and international level. Travelling to a customer abroad and meeting them may count as business activity and require a Business Visa and/or work permits. This is very relevant to Translators who are self-employed. Governments and military facilities are often interested in materials modelling, too. To work with such Clients the Translator may have to hold a passport of the respective country and require security clearance. Translators may also want to check if the country they are working from has an official ban on trade or other commercial activity with a particular country (embargo). If this is the case, they may not able to provide services.

Once the formalities are done, Translators can finally begin to understand the business case, based on their proceeding dialogue with the Client chairing the communication and appointing the subject.

Following the EMMC definition, understanding the business case means the realization by the Translator of the impact aspired by the modelling activity, including new innovative solution implementation, development of innovation potential of Client (SME or LE), profit, new market sectors opening, creation of new job places, economic and social benefits, development of new products or optimization of existing marks. Translators should discuss with the Client the expected outcomes and promote the success-line of the modelling project taking into account the real business situation by the Client, estimating risks and timeline.

The Translator should also list the benefits materials modelling can bring. A collection of qualitative benefits is provided by (Goldbeck & Court, 2016):

Materials Modelling can aid with …

- … more efficient and targeted experimentation
- … determining whether a target performance is easy to reach, just doable, or impossible
- … being a source of new property data
- … conducting a broader and more efficient exploration of new materials /processes
- … a novel corporate R&D strategy development
- … obtaining a deeper understanding of materials/processes
- … trouble shooting
- … performance optimisation
- … underpinning intellectual property (IP), supporting patents and in cases staking a wider claim
- … value chain benefits
- … improving collaboration and communication between R&D and production
- … upscaling and market introduction benefits

The Translators certainly may not overwhelm their Clients with all benefits at once, but rather select a few and adapt them to the business problem/challenge at hand. ITAINNOVA (Laspalas, 2016), for example, uses a conceptual classification of their type of Clients since the solutions they provide are different depending on the type of Client and can being tailored to their needs.

Often, Translators will not work directly with the Client they spoke to in the first instance. They may be appointed to work with a project manager, in particular, when a company has a high modelling maturity (Goldbeck & Simperler, 2019) and a process in place where all activities need to be accounted for. The Translator will not only have to suggest workflows, people and tools but also estimate how long all activities may take. The project manager has to provide a timeline to their superiors and estimate the costs *a priori*. People and tools can be in house, but if they have to be hired or purchased, new activities have to be added to the project and budgeted for. Also, new software tools require onboarding, and time has to be accounted for that. Project managers are usually very skilled in budgeting and time management, but the Translator has at least to aid with and often also allot where resources are coming from, how much they will cost and how long it will take for a modeller/modelling team to get up to speed.

The Translator, favourably, will have to have an insight into risk management. All materials modelling projects are inherently risky as they are novel and they may not deliver definite results due to their experimental or developmental nature. One simply does not know beforehand what the results are and how useful they may be. If the Translators suggest a well validated and verified workflow, the risk may be low. If they suggest a novel approach, the risk may be high but could maximise opportunities for the project at hand. In short, risk management aims to exploit or enhance positive risks (opportunities) while avoiding or mitigating negative risks (threats). Thus, the Translator should provide a list of risks[15], i.e., events that may occur and jeopardise the successful application of materials modelling. These could range from insufficient amount of data to failing to validate software. What will be needed is an estimate how likely risks may occur and suggestions for mitigation. A good

[15] https://prince2.wiki/theme/risk/

tool to assist here is a SWOT[16] analysis (Figure 5) (Madsen, 2016), which can aid to assess the Strengths, Weaknesses, Opportunities, and Threats one may encounter during a materials modelling project.

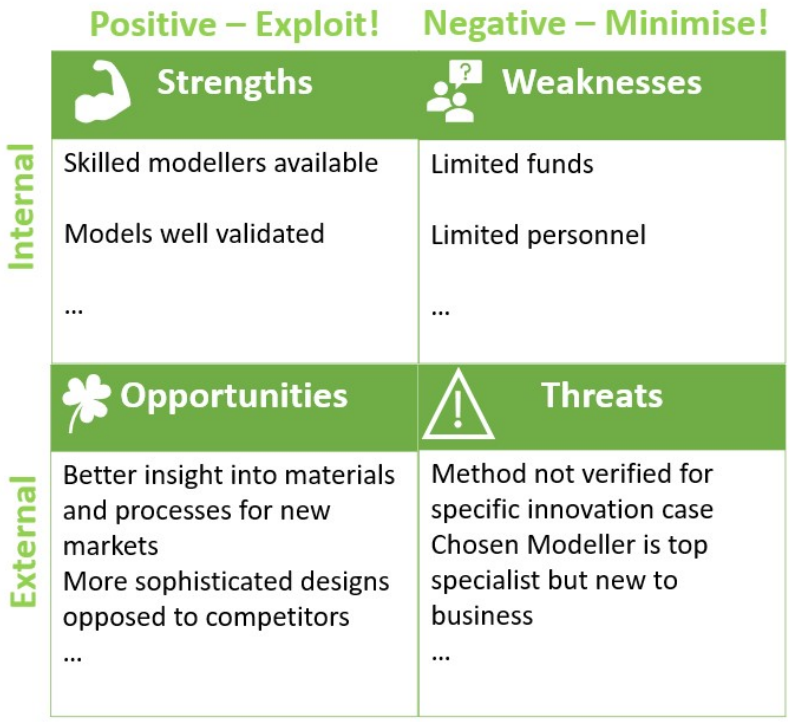

Figure 5. Example of a SWOT analysis for materials modelling in an industrial environment

Working step-by-step within a managed project with several milestones may seem to be restrictive at first for a very creative Translator but it can be very beneficial to document the process of modelling. Thus, materials modelling will become visible to more senior personnel in an organisation. Hence, it is recommended for the Translator to work out criteria by which the success of modelling can be judged by. Each well managed project should have a post project assessment and it is advisable for the Translator to compare projects with modelling to past projects without modelling and analyse the difference it made. The latter cold be done using tools like Return on Investment (ROI), see Appendix 1.

Translators are not only confronted with project management but also with novel tools such as Business Decision Support Systems (BDSS) and emerging Open Translation Environments (OTE)[17] such as OntoTrans[4]. For those, additional skills are required knowledge are discussed below in Chapters 4 and 5, respectively.

[16] https://www.mindtools.com/pages/article/newTMC_05.htm
[17] https://ec.europa.eu/info/funding-tenders/opportunities/portal/screen/opportunities/topic-details/dt-nmbp-10-2019

3.2. Step 2: Good understanding of the industrial case

It is very important for Translators to recognize where and what exactly the material or process related industrial problem is because the project pursued by the Client profits from division of work. Which technical specifications and regulations play a key role for the specific problem or industrial challenges? Are material or processing related issues the core of the Client (manufacturing and product lifecycle-related) interests? These factors affect to find or resign the industrial problem optimal solution and form the basis of the EMMC definition of good understanding of industrial case. In the realm of a "business case" one looks into business, i.e., a relation to the external world. When on then applies a business case internally in their organisation, we have reached the realm of the "industrial case". For the industrial case the innovation challenge framed by the business case applies. The material-related innovation challenge corresponds to the assessed industrial problem that arises from an expressed industrial need. Following DIN EN ISO 9000:2015 innovation is achieved by a new or changed object realizing or redistributing value. Relevant objects in this context are material products, processes, systems, or resources. The data that are relevant for the industrial case are facts about the assessed object.

When giving a modelling task for providing meaningful data or information, industry contacts will speak in natural language, will share their problem and will try to convey their challenge to persons acting as Translators. Thus, the Translator has to transform the information from natural language to "modelling" world (Figure 6)

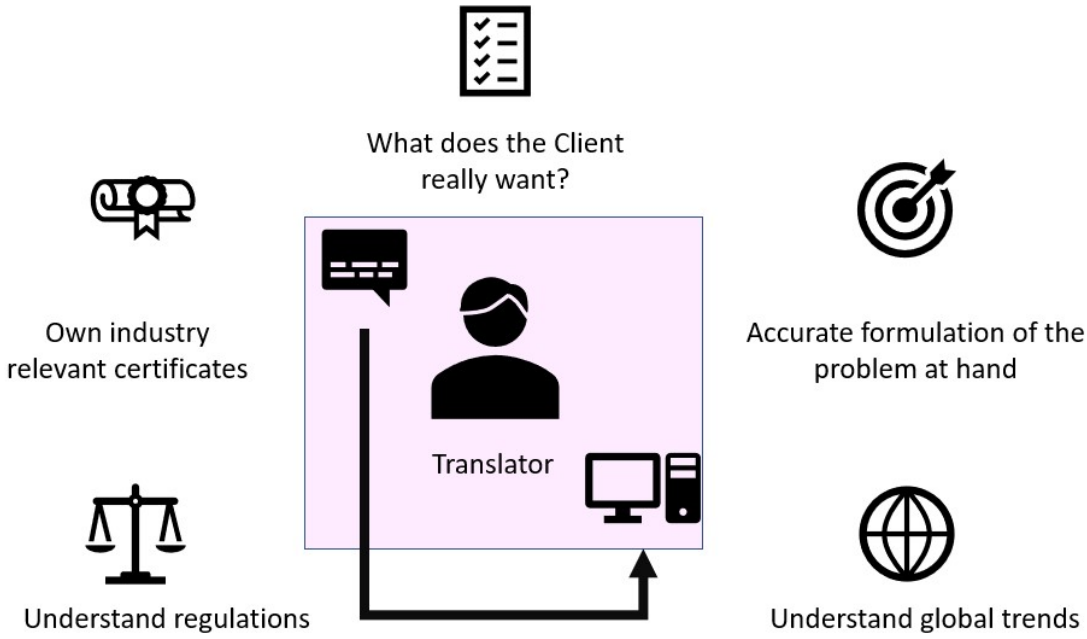

Figure 6. The Translator and their Clients– Translation from "natural language" to "modelling".

The Translator could be invited to work with Quality Function Deployment (QFD), which was developed in Japan in the mid 1960ies. The idea is to let the Clients express their needs or desires in

their own words and subsequently translating them into measurable product quality characteristics and/or further processing. (Barad, 2018). A Quality Function Deployment matrix can be built which is referred to “the House of Quality” (Hauser & Clausing, 1988). A good example on how to create one is discussed by (Lucidchart Content Team, 2019). Thus, from this matrix a Translator could see a Client’s needs linked to engineering characteristics, a more technical specification of a design/product. The latter can be used by the Translator as a valuable information to decide where materials modelling can have an impact.

If the Client is well versed and has worked with a modeller or Translator before, they can pose concise questions. These are highly technical to start with, and aim to find help through cooperation with materials modelling experts. Thus, the Client in this case seeks a particular service to an often business-critical matter. They may come across tense and urgent and require a Translator to find a fast, reliable solution rather than solely a component-based experimental and prolongated one. Translators who specialise in this type of problem solving to provide the focused project contribution should be well versed and well prepared in a range of available solutions and be able to think on their feet.

In this first meeting the Translator will be confronted with industry cases such as:

- The Clients want new materials, cheaper, but with better quality or sustainability than the current ones.
- Why is the Client’s material not working or no more compliant?
- From a list of possible materials or material combinations, which one should the Client choose?
- The Client perceives a process-related challenge (e.g., in manufacturing) that may be related to process planning, ongoing process qualification, preproduction series, or to urgent manufacturing issues. Which is the most sensitive process parameter in the layout, which material property makes that parameter so sensitive, and what is the material-related trend if some parameter tune-up is changed forward or backward?

What the Client really wants is to produce a product, and the Translator shall identify, substantiate and remove the obstacles to get there. It is of importance that the Translator knows the business and manufacturing around a material. Thus, somebody with experience in drug design is ill-suited to advice a Client on novel catalytic materials and their behaviour under real life respectively in-situ conditions. Expected though possibly not advisable answers to the questions above may be:

- Pick material X, it is better than the current ones; you can produce it and replace the materials currently used.
- Your material does not work because of Y. This is the way to overcome your problem and your product can work now.
- Choose Z. It is perfectly suited for what you try to achieve.

This is where the Translator has to be careful: major concessions are unprofessional. It is good practise to revisit the questions of the Client and formulate them in such a way that materials modelling can find the answer. Customer expectation management is key. For example, a Translator can tell the Client that they will be able to explain why a material does not work in a given application considering demands like the expected load or environment. However, there will be no answer which materials will work how much better. Indicating process-related trends (changes of material properties related to changing process properties), e.g., sensitivity or transfer function analyses, may be less timely and more efficient than re-iterating some already performed material development.

In case, the Client has only heard vaguely about materials modelling the Translator will have to aid/entrain them with asking the right questions. One of the main things to find out will be whether a problem is related to finding a new material or improving or describing the properties of a known material. It may also well be the case that industry is satisfied with the materials but would like to improve their processing or boundary-driven interactions with media. All of these may require different modelling expertise. The Translators should also manage the Clients' expectation as some modelling approaches are of an experimental and developmental nature. Similar to experimental assessments, not all approaches will lead to the wanted outcome but will provide quantified findings rather than logical yes/no ones.

Each industry sector has strict (regional) technical specifications, e.g., health and safety obligations, and every workflow suggestion has to be within those. It is worthwhile for the Translator in materials modelling to verify these together with the Client when discussing their problem. The translator may have to offer professional certificates to work in a certain industry sector. What would be necessary here is for the translator to verify technological competence in order to work in a particular industry. For adhesive bonding technology, the personnel-certifying, internationally recognised qualification "EWF-European Adhesive Engineer - EAE" is an option. This qualification is offered worldwide by Fraunhofer IFAM[18] and others, and serves as a recognised proof of competence according to Quality Assurance (QA) standards such as DIN 2304, DIN 6701 and TL A-0023 (German Bundeswehr/international requirement) and in future according to CEN (EN 17460) and ISO (ISO 21368). This can be helpful when working in Germany, Europe and beyond as exemplified by FEICA[19] (Federation of the European Adhesive and Sealant Industry, a multinational and member-based, value-oriented organisation representing the European adhesive and sealant industry). It is the responsibility of the qualification holder to check whether the official qualification is also valid in countries outside Europe. In any case, the qualification holders have to prove by which further training measures they keep their competence up to date Often, certificates may have a limited validity and require either refresher courses or recurring exams.

Translators have to be aware that decisions may have been made that they cannot influence but use as a specification or requirement. For example, an automotive manufacturer plans a "facelift"[20] for their cars and has already made a decision, how the design should look like. Thus, the novel material will have to fit the design. Prospectively speaking, the next facelift might then involve materials modelling already in the planning or concept phases.

The industrial case is often not restricted to the manufacturer but to global developments such as the European Green Deal[21] or the EU Circular Economy Action Plan[22]. Thus, industry have not only the challenge to drive innovation but are also driven by their ambition to keep a low carbon footprint and make their products recyclable. Industry will expect a Translator to support them in finding solutions for their respective all-inclusive or bite-sized challenges. For example, the study "Circular Economy and Adhesive Bonding Technology" by Fraunhofer IFAM (Mayer & Gross, 2020) describes the role of adhesive bonding technology in the context of the circular economy and places it in a political framework from a global and European perspective. It is recommended for Translators to collect

[18] https://www.weiterbildung.ifam.fraunhofer.de/en/adhesive-bonding-technology/european-adhesive-engineer.html
[19] https://www.feica.eu/information-center/education
[20] A "facelift" in automotive industry means that a car will have a noticeably different look than a previous year's model, along with updated features and new equipment.
[21] https://ec.europa.eu/info/strategy/priorities-2019-2024/european-green-deal_en
[22] https://ec.europa.eu/environment/circular-economy/

relevant studies pertinent to their field as their Clients may expect them to know about future perspectives and developments.

3.3. Step 3: Analysis of the experimental (and modelling) data available within the Client

To execute the modelling activity support, Translators need to analyse data (Figure 7) which are available for model input and validation. Moreover, they should be sure of the quality and accuracy or uncertainty of this data. If data is not available, incomplete or precarious, Translators should provide a strategy to approach the necessary parameters or propose "dedicated experiments".

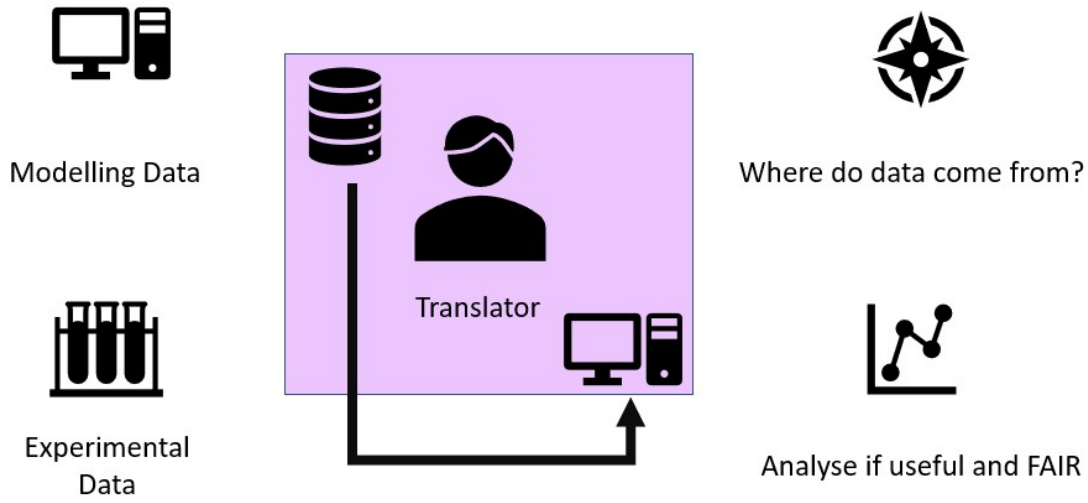

Figure 7. The Translator and useful Data, Translation from "Data" to "Modelling"

At this point, at the latest, the Translators will have to sign a contract/agreement with their Client as it will be necessary to look into available proprietary data. Some will be needed to identify relevant parameters and create an input for a materials modelling tool and some will be needed to validate or benchmark the results. Thus, Translators should be familiar with experimental data, characterisation methods and procedures performed in their respective field or collaborate with persons who have this expertise.

This step is very important for the Translation process, so Translators have to be as thorough and perspicuous as possible to extract from their Client all this information that is relevant for finding the solution efficiently and effectively. Project partners, both Clients and Translators, are often not very amenable to crude interrogation techniques, so tact and intuition (soft skills) will be key.

The existence or non-existence of data will most certainly influence the choice of workflows. The Translator should ask for data management plans (DMP) and check/assess with the Client the quality and accuracy/uncertainty of data. It is worthwhile to investigate if data are consolidated into a single consistent searchable format or if work has to be added to make data FAIR (Wilkinson & al., 2016), i.e., Findable, Accessible, Interoperable and Reusable. If this is not the case, the Translator may look into engaging with internal and external experts to rectify this. However, this could involve substantial

additional costs and invest for a Client. As this may not be always possible, the Translator will have to find solutions with what is available and both minimise and communicate the handicap on the quality of the modelling output.

It is unwise to use incomplete experimental data sets of low quality to validate materials modelling. The Translator can propose "dedicated experiments" to obtain more accurate data or suggest a suitable external database.

It is wise to produce a report for this step and document which metadata and data[23] and what sort of information was shared. It also should be documented if a Client or colleagues did not come forward with data or a suggestion to amend data was declined. This report can be seen as a protocol to capture the existence, origin, quality and missing data. Ideally, the Client will go through this protocol with the translator and confirms the content. This protocol will then serve the Translators to suggest workflows and come back to if they are asked by Clients why they have suggested a workflow. Organisations that offer Translation services may have similar procedures in place, hence the Translator shall follow these.

3.4. Step 4: Translation to (preferably more than one) modelling workflow

The neutrality and four-eyes principles and Client interests should be in focus and direct the Translator's choice in suitable modelling workflows for a particular problem. The specifications of different potentially useful models and software tools should be selected considering their availability, suitability, efficiency, and accuracy. User friendliness and reusability could be a significant parameter for SMEs. Moreover, validation of the model is important. The available experimental data and generation of new data should be taken into account for the recommendation of a workflow for the end-user.

From the other side, Translators' actions are based on the Client's experience and preferences in the modelling and simulation tool choice. In any case, Translators need to provide good and objective argumentation for the proposed modelling workflows. Of course, costs, general investments, simulation time and level of maturity play an important role in the modelling tool choice. However, a return on investment (ROI) and benefit analysis can help Translators to facilitate a Client's decision making.

Once the information is in place, the Translators suggest several modelling workflows, i.e., they translate their modelling idea into actual workflows (Figure 8). The Translator may want to consider, if the Client already owns software and if the task can be done with it. Also, if new software will be needed and if it can be compatible with the tools the Client already owns. If the Client is new to software, solutions like Software-as-a-Service (SaaS) or Modelling-and-Simulation-as-a-Service (MSaaS) can be considered.

[23] "Data" shall mean metadata and simulation/characterisation data throughout the manuscript.

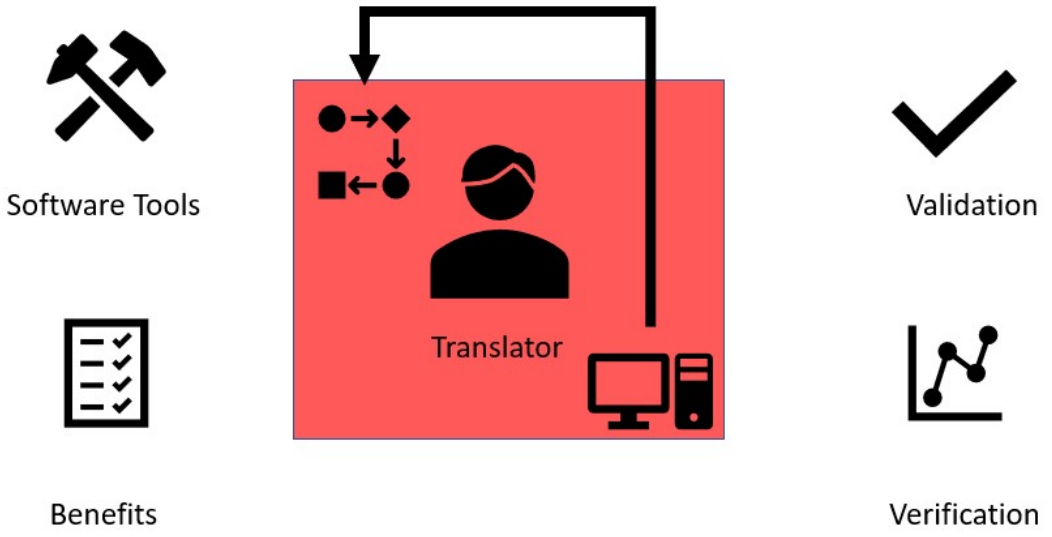

Figure 8. The Translator and Workflows, Inverse translation from "modelling" to "workflow"

The workflow aims at providing relevant data/information or required insight to the Client. The EMMC would recommend as a good way to record a modelling workflow to use the MODA[24] (CWA 17284, 2018)(de Baas A. F., 2017), including a flowchart (Figure 9). Such high-level analysis of workflows provides an efficient way of discussing and capturing different approaches.

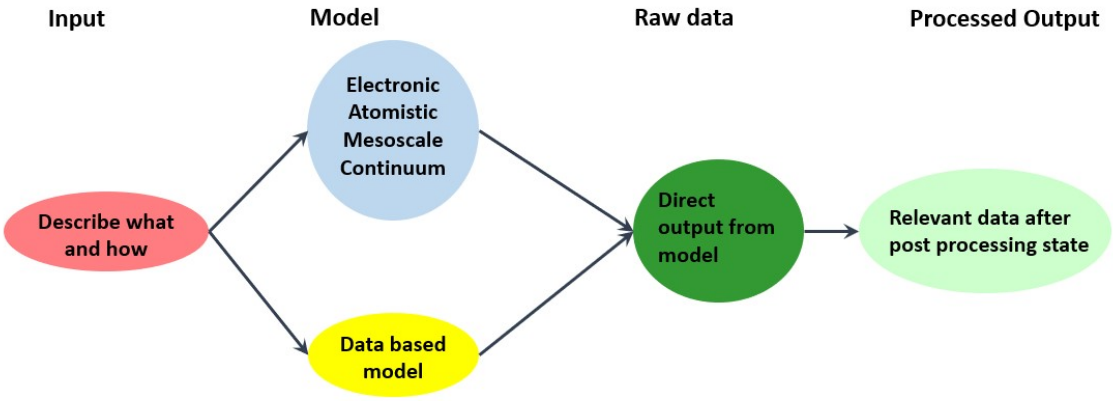

Figure 9. Schematics of a MODA flowchart

In Figure 9, the pink bubble incorporates the framework involving the findings in step 1 and describes the actual input required for a workflow like a structure, parameters added to a GUI, etc. Materials modelling can involve electronic, atomistic, mesoscale or continuum modelling or even multiscale approaches (de Baas A. F., 2017) and the blue bubble will host information about them. However,

[24] MODA – Modelling Data Tables.

data-based models (like machine learning, A.I.) may be considered as well and in this case, a yellow bubble will replace the blue one and comprise information about the recommended and finally used model. The dark green bubble describes the actual outputs that a software tool produces. These are rarely useful, so a postprocessing step such as visualisation of a field or plotting graphs, etc. may be added and documented in the light green bubble. This can happen along with the respective data documentation in materials characterization (Romanos, et al., 2019) and that will be the base for the following steps of the Translation process.

The Translator should objectively suggest models and software tools and rate their suitability, efficiency, performance and level of maturity, comment on their user friendliness and model accuracy or predictability. The jargon used should match the Clients' experience (Laspalas, 2016) and to enable them to consent to a chosen workflow and tools. The Translators and their Client should agree on a workflow.

Once the Client agrees on a workflow, the Translator will estimate costs such as investments in person weeks/months, software, hardware, simulation time, services, etc. If the Client requires some metrics, the Translator could calculate return on investment or analyse the benefits. (Goldbeck & Simperler, Strategies for industry to engage in materials modelling, 2019)

The used models have to be validated and verified (Ryan & Wheatcraft, 2017). Hence, the Translator has to provide strategies to show that the model is fit for purpose (verification) and produces reliable results (validation). Data and information on materials modelling software tools may be found with software owners or in peer reviewed literature. If not, we suggest to the Translator to orchestrate a "proof of concept". Hereby, experimental data are used as a benchmark for a small test project before the Client commits to the full project. This will be done by whoever conducts/provides the modelling work and monitored and assessed by the Translator.

Validation and verification are very important for multiscale models, as one has to understand how exactly they communicate and how numerical errors propagate from one model to the next. (Hoekstra, Chopard, & Coveney, 2014)

The Client may also profit from less technical analysis, such as a benefits assessment of different workflows and a qualitative judgement of the underlying technology. For example, we could describe workflow one as fast, less accurate, but well validated; workflow two as time extensive, highly accurate and well validated. Workflow three however could be cutting edge science, medium time effort and not validated. Hence, the Client knows better how involved and reliable the different options may be.

3.5. Step 5: Propose the Client modelling executor(s) and strategy for model validation

The Translator is expected to have an extensive network of persons/institutions who are capable of performing the actual modelling and an in-depth knowledge on software tools. Thus, they are required to update themselves regularly on publications highlighting excellence or novel developments on the software market. It is an impossible task to master all available software on expert level and to keep up with all newly developed features. It is more realistic though, to monitor the persons who are the experts and tap into their knowledge and skills.

Here, the Translators talk to their peers using “modelling” as the *lingua franca*. (Figure 10)

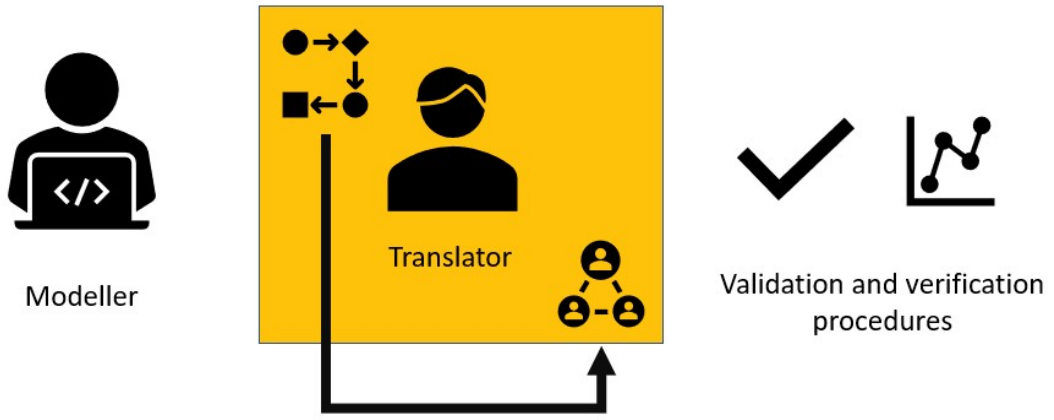

Figure 10. The Translator orchestrates and facilitates materials modelling, they convey the workflow to a peer, speaking “modelling”

To convey the idea even better, why in a Translation process a Translator should not act as a member of the modeller team, we will draw an analogy to the setup of a Trauma Team (Tiel Groenestege-Kreb, van Maarseveen, & Leenen, 2014) and the interwoven process steps in hospital emergency rooms. Studies show that when a team is formed around a command physician/surgeon this allows for distribution of several tasks in assessment and resuscitation of a patient in a ‘horizontal approach’, which may lead to a reduction in time from injury to critical interventions. The team lead checks that all is proceeding satisfactorily and all tasks are executed by skilled staff. In their more strategic role, the team leaders can formulate a plan for the post trauma treatment which will be in the best interest of the patient.

Translators can be seen as the strategic lead in a horizontal modelling approach and advise also who shall take on the different roles. They should suggest a modeller based on their expertise, experience, availability and the Client’s preference if they have any. By not performing the roles themselves they can follow the project execution and assess the progress and represent the Clients’ interests better. Before the modelling happens, Translators will also have to strategically plan how their chosen and applied model can be validated. Not only will they have to orchestrate the modelling but also function as an ambassador for it and tell their Client why their choices are of value. As the modelling happens, Translators have to put the validation into execution. Translators follow the project execution and represent the Client interests face to face with the modeller.

Another reason why a Translator and the modeller should not be the same person, can be explained with the Four-eyes principle (Kytová, 2019) in language translation. Hereby the roles are “Translator” and “proof-reader”. If we transfer this to our subject, the modeller is not only the executor of a workflow, but may also serve as a sparring-partner to discuss a workflow in detail. We are aware that in some business setups this separation may not be possible, but we advise a Translator in such circumstances to find a pair of fresh eyes to look over a workflow, strictly compliant with any NDA that was signed.

However, being a Translator is performing a role – and as such this role is in principle exchangeable. It could well be, that a Translator becomes a modeller in another project, and another qualified colleague or business partner takes over as the lead.

3.6. Step 6: Translation of the modelling results to information that is understandable, reliable and usable by the Client

Translation is not a one-way street; once the results are obtained from materials modelling, the Translator must establish the relationship of the results to the challenge and the question the Client had (Figure 11). A follow-up, evaluation of the process, interpretation and formulation of recommendations for the Client are strongly recommended for rounding off the personal dialogue(s) engineered/initiated in steps 1 and 2. This task can also be done with the modeller, who conducted the research. Naturally, Clients who are familiar with modelling may be able to interpret modelling results by themselves.

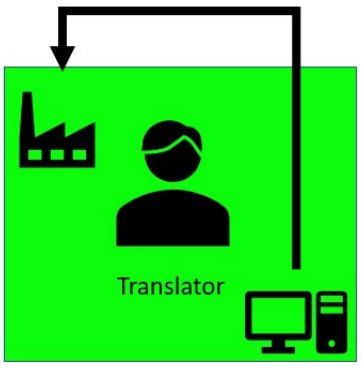

Figure 11. Inverse Translation from "modelling" to "business"

However, we would recommend the Translator to offer and schedule such services to make sure the results are well understood. Preferably, this manifests in a report that can be entered into a project management system where other stakeholders of an organisation can peruse it. Furthermore, the Translator can assist the Client to identify the acceleration points, i.e., where did modelling bring a benefit. Sometimes, experienced Translators can foresee the additional perspective for the business development, which can help to build the long-time collaboration and strengthen the trust between the Client and the translator. Moreover, based on the project results and the inverse translation step the "track record" of expertise on Translation could be prepared. At the same time, the confidentiality of the project related information and data create problems to prepare and publish the open Translation documentation. Translator should discuss and approve with the Client a possibility to collect and publish the Translation cases to use them for their successful professional development and career.

In a nutshell, following the sequence of steps 1 through 6 the Translator will not only provide relevant answers to focused questions asked by the Client based on their challenges but also a concise project documentation.

4. Translation when working with a Business Decision Support System

In general, a Business Decision Support System (BDSS) is a system in an organisation to take informed decisions across its different operations. Here, we refer to BDSS in the context of materials modelling, as was elaborated in (Dykeman, Hashibon, Klein, & Belouettar, 2020). Under the umbrella of the EU programme NMBP-23-2016 [25], two such BDSSs were developed, COMPOSELECTOR[26] (Belouettar, et al., 2018) and FORCE[27]. These materials modelling based BDSSs are designed to combine materials models with other sources of information and turning it to actionable knowledge that drives business decisions based on selected Key Performance Indicators (KPIs). This means, the Translator will have to understand business concepts in depth (Figure 12) to provide a translation fit for a BDSS. Notably, the primary handler of the BDSS is a decision maker, not the Translator.

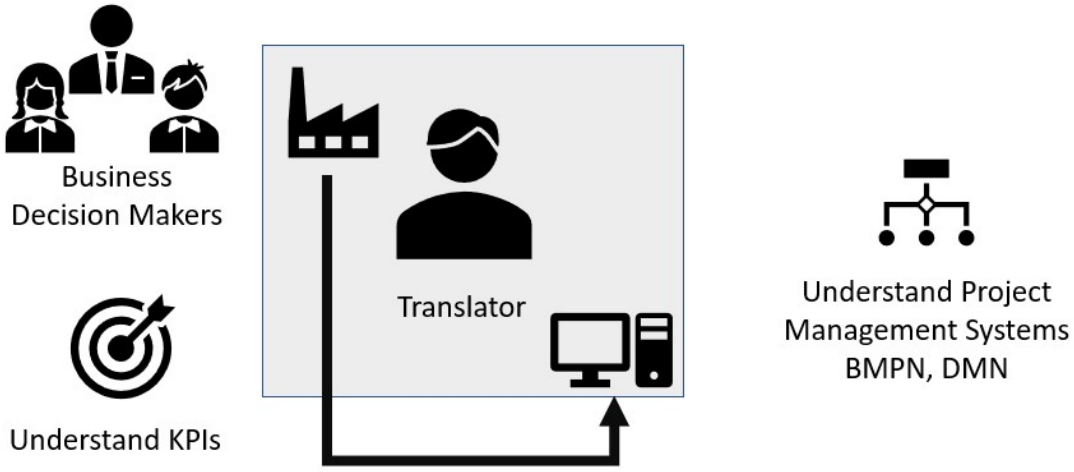

Figure 12. The BDSS Translator

Business Process modelling may be already in place within an organisation and a standard Business Process Model and Notation (BPMN) is often used. [28] For the decision-making part, the Decision Model and Notation (DMN)[29] can play a role. We expect, that a team of translators will engage with a Client,

[25] https://cordis.europa.eu/programme/id/H2020_NMBP-23-2016
[26] https://cordis.europa.eu/project/id/721105
[27] https://cordis.europa.eu/project/id/721027
[28] https://www.bpmn.org/
[29] https://www.omg.org/dmn/

where some persons are fluent in business modelling and some in traditional translation, as described in Chapter 3.

In order to enable an analysis that connects the Translators' activities 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 13).

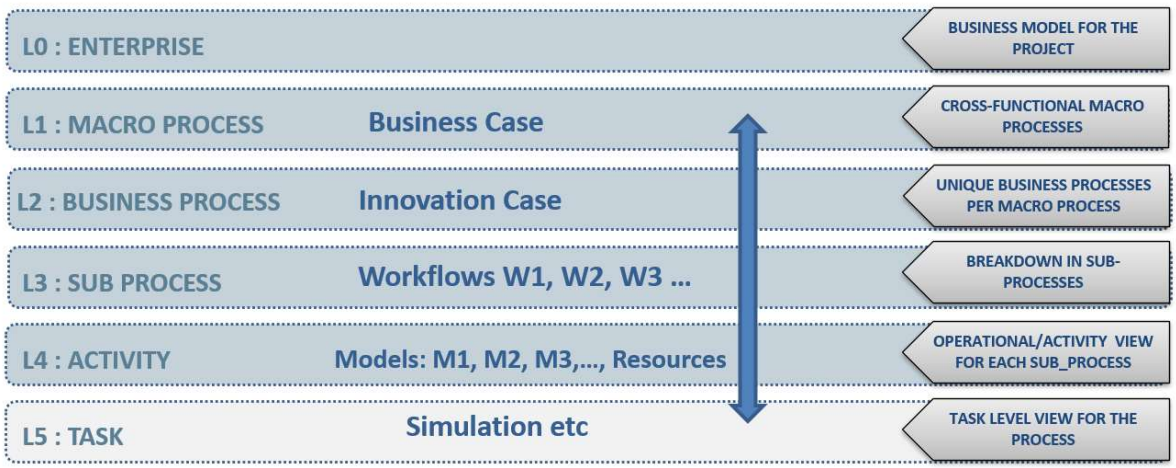

Figure 13. Six levels of a generic business processes with a blue double arrow marking the involvement of the Translator when using a BDSS.

The Translator enters the business processes on the Macro Process Level and needs to suggests tasks. Thus, Translators will have to work intensively on Step 2 (Chapter 3.2) and understand the business case and identify and quantify the true benefit to the Client. A good source of information that will aid a Translator to understand BDSSs better can be found in a recently published guideline (Dykeman, Hashibon, Klein, & Belouettar, 2020) by members of the COMPOSELECTOR and FORCE projects. The Translators need to use the sequence discussed in this guideline and use the six steps of translation to follow it through.

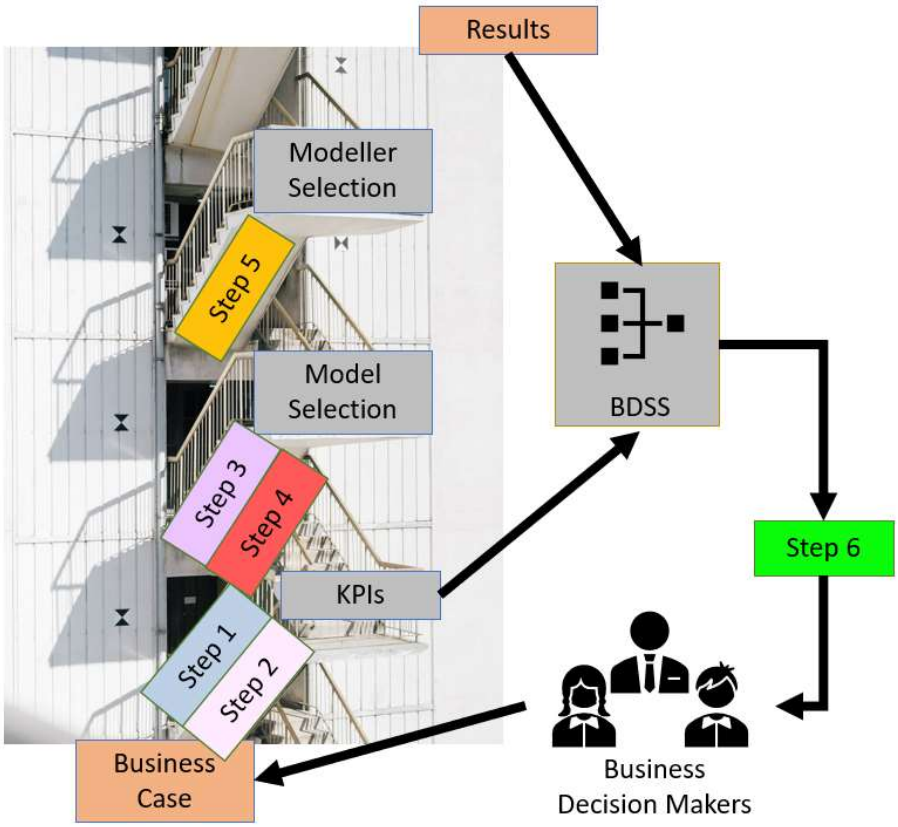

Figure 14. The grey boxes depict the sequence of some of the BDSS translation tasks as described in (Dykeman, Hashibon, Klein, & Belouettar, 2020) and the "Step boxes" describe the Translation steps (Chapter3) needed to follow the sequence.

We will discuss how to apply this to a widely published industrial case example (NIST, 2016), QuesTek's Ferrium® M54® [30]steel for application in U.S. Navy hook shanks. Th objective of the U.S. Navy was to develop an improved alloy at a lower cost than current materials which is the business case, see bottom stair case of Figure 14.

Industrial Case Example

QuesTek[31], a US based company, deploys its metallurgical expertise and Integrated Computational Materials Engineering (ICME) technologies to assist with materials-related technical challenges. Prior to Ferrium M45, they developed Ferrium S53 alloy, which offers ultra-high strength, high toughness, corrosion resistance and it is being used without toxic cadmium plating in e.g., landing gear. (Olson, 2013) describes in his paper, how materials modelling was harnessed to design a ferrous alloy which could then be used in a real-life application. A big advantage of ferrous alloys is that their microstructural phenomena are well understood and were validated with fundamental experiments. Olson showcases in his paper, that in depth knowledge of the material *per se*, and the processing it undergoes is key to understand how it performs. Figure 5 in (Olson, 2013) depicts how processing influences the structure of a material, and subsequently its properties. Of interest are strength, toughness, and resistance to impurity embrittlement and an ICME approach leading from electronic to continuum models was introduced in (Olson, 1997). To reach TRL 7, where Ferrium S53 was part of the landing gear of a test flight, took 8.5 years.

[30] https://patents.google.com/patent/US9051635B2/en
[31] https://www.questek.com/

For Ferrium M54, QuesTek provided their materials and process design expertise and also took on the overall project management. If we match their role to our translating process, the US Navy would have the role of a Client, and QuesTek provided the Translators, modellers and project manager.

In the following section we will use information from (NIST, 2016), (Olson, 2013), and (Olson, 1997), and match it to the BDSS procedure. In this hypothetical scenario we will retell what would have happened, if a BDSS was used and generalise by calling QuesTek "the Translator" and the US Navy "the Client".

The Translator interviewing the Client may have used a mixture of actions described in Steps 1-2 to deduct two high-level attributes, "improved alloy" and "lower cost". "Improved" can mean many things. This is where the Translator has to ask further questions. The Client could give more details: ultra-high strength and toughness were the attributes they were after and lowering cost meant also to reduce the amount of coupon testing and a longer life span. This will lead the Translator to formulate the actual KPIs.

The KPIs could be for example:

- Cost saving, measured in US$
- Lifespan, measures in units of lifespan of old hook materials
- Fracture toughness, changes to or range, measured in $MPa \times m^{1/2}$
- Tensile strength, changes to or minimum, measured in Pa

These KPIs have then to be logged into the BDSS. The translator could then collect data form their Client who had requirements what properties a hook shank needs to have to comply with regulations. If the Translators have proprietary databases, they could add to the data collection (Step 3). The models used for the calculation of microstructure formation in time and space could start on the electronic level followed by continuum mechanics (Step 4). Step 5 would then engage modelling specialists. However, step 6 is now taken on by the BDSS. The system does the backtranslation for the Translator and "climbs" the stairwell (Figure 14) down again aided by powerful decision tools such as multi-criteria optimisations. The reverse steps are:

- Calculations of microstructure formation in time and space for several alloys.
- Toughness and Strength are reported.
- If they fit the given range, the alloys pass.
- Lifespan and Cost savings are estimated.
- The alloys that fit, pass.
- The Client/decision maker gets a list of alloys that fit the criteria, and thus can decided which alloy makes it to production.

5. Translation in the Context of the OntoTrans Open Translation Environment

Translators working with the OntoTrans OTE will utilise semantic technologies to support the translation process and may require relevant skills (ontologies, working with knowledge graphs, etc.) in their team. The Horizon 2020 project OntoTrans[4] started in April 2020 and work is planned to train internal Translators on how to work with an OTE and enable them to embrace translation in a more holistic way. Hence, this chapter will introduce the vision that the OntoTrans partners have for this role.

The Clients are expected to define an Innovation Case, often aided by a translator, and they are looking at Level 2, having gone already beyond the macro process. (Figure 15)

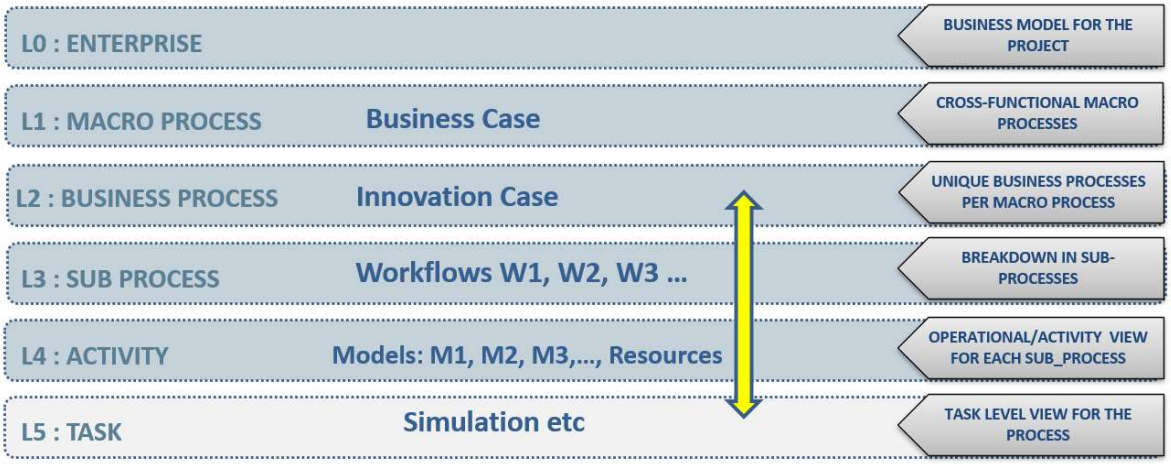

Figure 15. Six levels of a generic business processes with a yellow double arrow marking the involvement of the Translator when using OntoTrans

The Client has to become very involved and invest in using ontologies. Thus, we envisage a team of data scientists and internal translators to support the setup. The OntoTrans system provider will be working with the Translator (often company internal) and the end user Client (Figure 16), to go from Innovation Challenge to the Innovation Case and potential MODA type workflows.

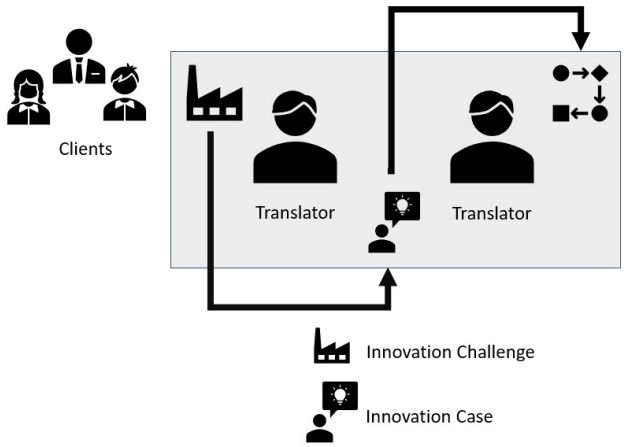

Figure 16. OntoTransLator: Business to Workflow

They then join forces with a data scientist to build the ontology and knowledge source connections and providing the company internal Translator with interfaces (i.e., software wizards that guide through the translation process). (Figure 17)

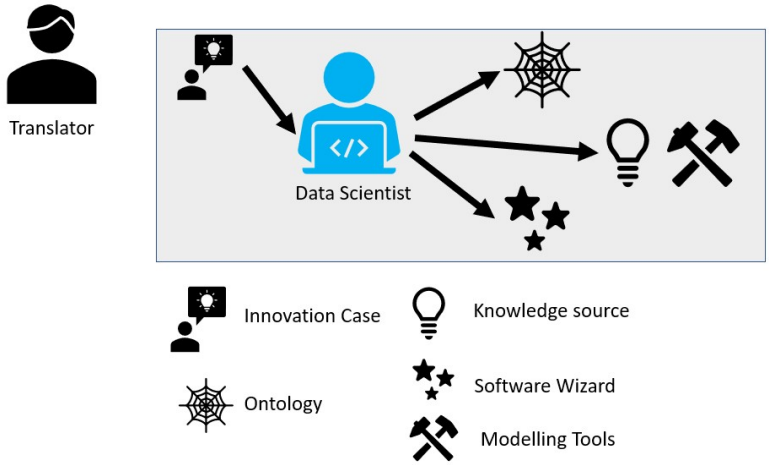

Figure 17. The OntoTransLator and the Data Scientist

There will be two scenarios for OntoTrans, which are the setting-up and the day-to-day use:

Scenario 1: setting up a versatile OTE ("for the very first time") is time-consuming and needs to involve several roles provided by a team of experts;

Scenario 2: re-using a once established/appropriate OTE that already is filled with default settings for potential new innovation cases; Once the OntoTrans implementation is up and running, we can envisage a Translator to explore potential solutions and do data analytics with the Client. That will typically be a company internal Translator.

A high-level overview in Figure 18 shows schematically what this OTE may look like.

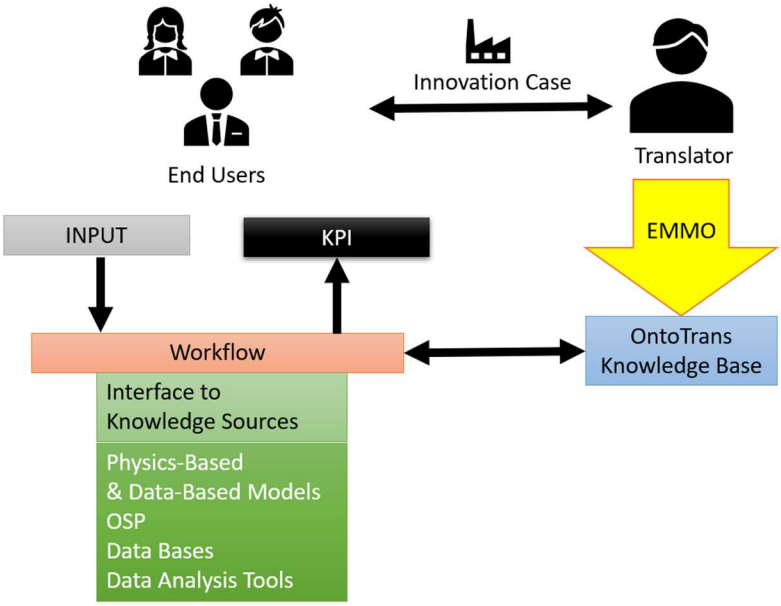

Figure 18. Schematic Representation of OntoTrans

The Clients/End Users present an Innovation Challenge and express in natural language the high-level objective, e.g.

- The Client needs to master their process parameters better
- The Client needs to improve their agile response to product/market/regulatory requirements
- If the Client improves their product, do they sell more?

We will use again the case study by QuesTek (NIST, 2016) and will retell, what hypothetically could have happened, if OntoTrans was used.

The Client wants to know: "How can I get a more cost-effective alloy with a certain fracture toughness and tensile strength that has double the life time of a hook we are currently using?" The translator will use Step1 and Step2 to extract all information from their Clients to cover all properties and processes relevant to their Innovation Case. What is new is that the Translator will work with data scientists/ontologists to construct an application ontology or, preferentially, develop a domain ontology compliant to the European Materials & Modelling Ontology (EMMO)[32] to translate the real-world case into a language which is EMMO compatible (yellow arrow in Figure 18). This means all processes and properties around creating a hook from a new alloy must be found within the OntoTrans Knowledge Base, e.g., a hook is a Materials Object, it can be composed from an Alloy, it has this tensile strength and this fracture toughness, etc. There is a benefit of defining things at a meta level: if one connects the innovation case to certain types of properties, then one can connect any knowledge source that provides the property; hence any model, database, experiment that provides the property becomes in principle accessible to the Translator, once the system grows to include more and more knowledge sources. Step 3 will be used to find data (green-hued under knowledge sources in Figure 18) and link them to the OntoTrans tool via interfaces. Step 4 will be used to find modelling solutions (green-hued) and link them also via interfaces to the OntoTrans tool (blue-hued). Step 5 and step 6 will then be performed by the workflow the translator team builds (red-hued).

The Clients -wizard interaction could be imagined as follows:

Client	Wizard
Fills in values for tensile strength and fracture toughness	Searches database and offers a list of alloys
Demands life time of hook to be twice as long as currently used ones	Takes alloy compositions as an input and initiates calculation of microstructure formation in time and space
Browses through outputs and picks good alloy compositions for coupon testing	

[32] https://github.com/emmo-repo/EMMO

6. Discussion and Outlook

Translator is a role suggested and defined by EMMC with input from stakeholders, but not in any way an officially recognised occupation. However, the effort of the EMMC and the persons engaging stakeholders to join this bottom-up approach, lead to a viable process (6-steps of Translation) a Translator basically can follow. As stated above, not all steps have to be followed all the time. End-users in industry companies and organisations are given the opportunity to identify and contact Translators who are experts in Translation, modelling and come with dedicated domain-related competence. Exemplarily, customers may benefit from efficient and effective guidance provided based on the ontology-driven Translation router APP that is developed by the team of the Virtual Materials Modelling Marketplace (MMM) VIMMP. (Horsch M. T., et al., 2020) profiting from the MMTO (Materials Modelling Translation Ontology) developments. (Horsch M. T., et al., 2020)

Organisations with a high modelling maturity (Goldbeck & Simperler, 2019) maybe aware how modelling can help already, and engage with a Translator from Step 4 onwards. BDSSs have some sophisticated tools that enable a decision maker (maybe non-expert in materials modelling) to take some without the translator. For example, both FORCE and COMPOSELECTOR comprise both multi-objective optimization tools that consider multiple criteria, and deliver a preferred decision with ratings to a Client. This enables them to select an approach without asking a Translator for advice. Also, Step 6 is incorporated in the BDSS, and "the system" offers a translation of modelling results to an answer suitable for the Client to understand. However, a BDSS does not make a Translator in materials modelling redundant – it just evolves their role and entangles them closer into the Business environment. OntoTrans will ask the Translators to become more engaged with Ontologies and Semantic representation of innovation cases. The Translator will become some sort of a digital twin of themselves and serves their Client by creating and utilising Translation Tools in form of APPs or software wizards.

We are aware that in detail domain-specific translation is complex, imposing both communicative and technical challenges to the Translator. Innovation is intended to go beyond the state of the art in economic, ecologic and societal dimensions. For each business and industry case an individual superordinate innovation challenge is to be assessed. Still, we distinguish that both the usage of a domain-specific taxonomy and "view of the world" on the one hand and of largely harmonised intercommunity procedures when assessing business or industry cases on the other hand result in repetitive patterns for the translator work. Therefore, profiting from a monolithic and one-stop procedure based on a joint representational formalism will permit a translator significant time savings and translation quality gains. FAIR translation is facilitated by versatile application of top-level ontologies comprising material and process-related entities as well as business-related entities and their interrelations. With these being based on international standards, the compliance of an ontology with established harmonised procedures will facilitate a FAIR ontology-based approach that comprises interdomain commons and helps to greatly disburden the translator from.

7. Conclusion

Our whitepaper recapitulates and extends on the framework of a process called "Translation" in materials modelling which evolved over the last six years by consulting the different (European) stakeholder communities (Translators - individual and organisational, modellers both in academia and industry, software owners, and representatives of the materials and manufacturing industry). The six steps of the Translation process in materials modelling outline with graphical abstracts what the process includes. Translators could follow this Guide in dialogues with industry Clients and materials

modellers, respectively. The actual Quality Assurance (QA) is the responsibility of the Clients within their framework. Hence, we attempted to make the Translation process in Materials Modelling as transparent as possible, to enable a Client to assess it with their means. In this way, the Translator contributes to bridging the product and the entire industrial production chain, by tailoring modelling workflows providing meaningful data to industry Clients for supporting their business decisions.

The concept of Translation is further developed as a part of the EMMC Focus Area "Impact in Industry"[33] with the majority of authors being in active roles. It is pertinent, to have a common exchange platform to enable the role to evolve alongside new developments in the materials and manufacturing industry.

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Disclaimer

All information contained in this study and any opinions expressed in it are intended to introduce translation as a process to enable a better integration of materials modelling in industry and manufacturing. All statements of fact, opinion, or analysis expressed in the report are those of the authors. The information used and statements of fact made are not guarantees, warranties or representations as to their completeness or accuracy. The authors assume no liability for any short term or long-term professional decisions made by any reader based on analysis included in this report.

Acronyms

A.I. – Artificial Intelligence

BDSS – Business Decision Support System

BPMN - Business Process Model and Notation

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

COMPOSELECTOR - Multi-scale Composite Material Selection Platform with a Seamless Integration of Material Models and Multidisciplinary Design Framework.

CSA – Coordination and Support Action

DIN - Deutsches Institut für Normung e.V. is the German national organization for standardization and is the German ISO member body.

DMN - Decision Model and Notation

DMP – Data Management Plan

[33] https://emmc.eu/activities/emmc-focus-areas/impact-in-industry/

DVM - discrete variation method

ECCOMAS - European Community on Computational Methods in Applied Sciences

EMMC – European Materials Modelling Council

EMMO – European Materials & Modelling Ontology

FAIR – Findable, Accessible, Interoperable, Reusable

FORCE - Formulations and Computational Engineering

GA n. – Grant Agreement Number

GUI – Graphical User Interface

ICME - Integrated Computational Materials Engineering

IFAM - Institut für Fertigungstechnik und Angewandte Materialforschung (Institute for Manufacturing Technology and Advanced Materials)

IP – Intellectual Property

KPI – Key Performance Indicator

LE – Large Enterprise

MMTO - Materials Modelling Translation Ontology

MODA – Modelling Data

NIST - The National Institute of Standards and Technology

NDA – Non-Disclosure Agreement

OTE – Open Translation Environment

PDCA – Plan, Do, Check, Act

QA – Quality Assurance

QFD - Quality function deployment

R&D – Research and Development

ROI – Return on Investment

SME – Small and medium size Enterprises

SOW – Statement of Work

SWOT – Strength, Weakness, Opportunity, Threat

TRL – Technology Readiness Level

WCCM - World Congress in Computational Mechanics

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APPENDIX 1 - EMMC Translation Case Template

EMMC Translation Case

Introduction

Translator

- Name, affiliation and contact details
- What type of Translator is your institution: TTI (Technology Transfer Institute), Academic group, Software Company, Manufacturing Industry, Other (Consultancy, etc.)
- What is you field of translation expertise: specify type of material or type of models according to RoMM (please see (de Baas A. F., 2017))

Client

- Who is the Client? Is the Client a large company, SME or a consortium thereof?
- Which value chain segment (e.g., material producer, convertor, end-user) it is positioned?
- Did you have existing collaboration with the Client?

Industrial/Business Case

- Describe briefly the industrial problem.
- Indicate involved budget or preferred time to solution (duration).
- Indicate what was the expected outcome of the translation process.

Translation to modelling solution

- What type of model(s) did you use propose and use? Explain arguments and criteria used to propose and choose a specific modelling approach and modelling executor for the specific industrial problem.
    - Include inventory and data quality assessment. Was it necessary to realize dedicated experiments prior to simulation? Describe the required validation steps.
    - Were model accuracy and necessary investments discussed? If so – please describe.
    - Who made the final choice for the model and for the modelling executor? Based on which criteria?
    - Explain the involvement of the Client in the case.

Evaluation of the translation case

- Indicate eventual bottlenecks encountered in the translation process or any suggestion for improvement of the process.

Client's benefits from the modelling

- How did the Client use the modelling results?
- What were the benefits for the Client of using modelling?

Economic impact of the modelling project

- When possible, estimate the **Total Client Investment (TCI)** in this modelling project as the sum of all Direct Costs. Direct Costs are, for example: Software cost/ licenses, Hardware cost, IT support, Labour/ Material cost, Training, Staff cost, Computing cost.

Direct Costs	EUR

Total Client Investment (TCI)	EUR

- Estimate the **Total Client Benefit (TCB)** from this modelling project. Please consider certain KPIs (e.g., costs for saved number of experiments, cost for saved materials, costs for personnel saved for experimental work, improved processing etc. For more information please look at (Goldbeck, 2012)

Client Benefits (e.g., based on certain KPIs)	EUR

Total Client Benefit (TCB)	EUR

Return on investment (ROI)

- Calculate the ROI as a ratio of the Total Client Benefit (TCB) and the Total Client Investment (TCI):
  ROI= TCB/ TCI

ROI	