



Materials modelling criteria used by Translators

Translator survey

Natalia Konchakova, Denka Hristova-Bogaerds

EC workshop, 21 September 2017, Brussels





Aim of the Survey

Translators:

- EMMC Survey for model developers, software owners/engineers and industrial users of modelling **to define the criteria** that **translators** can use when selecting the most suitable model/software
 - **Model developers (modellers)** are expected/encouraged to provide:
 - Model validation cases/procedures
 - Accuracy (when possible to be evaluated)
 - Model specifics e.g. level of model maturity/development: new models (higher risk models) vs. more mature models (expected to have also more established validation/benchmarking procedures)
 - **Software owners/engineers** are expected/encouraged to provide:
 - Relevant (validation) case studies to demonstrate the accuracy of their software (such can often be found also in software manual)
 - Applicability and especially the limitation of each software
 - Upon specific request: round-robin tests by software users and model developers or additional demonstrations for specific industrial cases
 - Link to the Survey will be posted on <https://emmc.info/> with invitation to the modeling community to participate.





Survey structure

- academic model developer/user: questions 1 to 5
- software owner/engineer/developer: questions 6 to 9
- industrial user of modelling: questions 10 to 13

21 Participants:

model developer (MoDe)	9
software owner (SWO)	10
industrial user (InUs)	2





1. Please specify if your model(s) is physics-based model or data-based model

MoDe

- Physics - based model: 4
- Data - based model: 3
- Both: 3

Action for modellers and SWO:

- *Indicate the model as physics-based model or data-based model*

Action for Translators:

- *Use this specification as the first important model characteristic for Translator!*



2. Can you specify the level of maturity / development of the models you use/develop?

If YES – please list the levels of maturity of the models you use/develop and the criteria for their determination. If NOT – please explain why.

- No, I am a beginner - No, I am working with my first materials model ...
- Yes, we use different models at different maturity from academic model to Commercial software
- Yes. The Model is a quite consolidated models, as implemented in several commercial software available on the market

Problem: Definition of the maturity

Action for modellers, translators and industrial users:

- *Define the characteristics of model maturity*



3. Can you provide model validation cases / procedures and estimation of the accuracy of the models you use / develop?

MoDe

If YES – please give an example. If NOT – please explain why.

Yes:

description of relevant experimental techniques: 5

report of analytical approaches required for the model validation: 2

virtual cases used to evaluate the modelling result: 1

No: lack of the sufficient expertise in model validation

Action for modellers:

- *Describe the criteria or procedures for estimation of models accuracy/uncertainty --> Useful for translators and end-users*

Action for Translators:

- *Provide the training / workshop on model validation approaches*





4. Are you able to make a rough estimation on the cost/investments for performing modelling project,

MoDe

for example investments in person months and hardware, simulation time, software licences (if needed) etc.? If YES – please list the criteria you use for estimation of the cost/investments. If NOT – please explain why.

- Yes - Description of the potential cost/investments without the values: 4
- Yes - Rough estimation with values: 1
- No: 5

Why is it so difficult for modellers to evaluate the costs for modelling?

Action for Translators:

- *Provide training for modellers “Estimation of modelling project investments”*





5. Do you use/have other features of your model to profile it?

MoDe

- Create industrial focused models: 3
- Initiate the study of specific aspects of material behaviour: 2
- No: 4

➤ *The industrial application will make the models more “attractive” !*

Action for modellers:

- *consider applicability of your model for industrially relevant materials and processes*





6. Can you briefly outline the applicability (e.g. for which type of problem/material/process/property) and the especially the limitations of your software?

SWO

If YES – please describe briefly both. If NOT – please explain why.

Applicability – general descriptions, advantages, industrial orientation - ALL SWOs

Limitations – **only some** of the SWOs mention them: real limitation – 3;

- *Computation time; number of atoms validated for system; missing experimental data; mesh broking in specific case*
- *How to deal with confidential information from SWOs regarding the limited applicability of their software?*
- *How can we have the real picture on what is realistic to achieve at the moment with certain software?*

Action for SWOs and Translators:

- *Work together to try and list as concrete as possible the realistic application of the software tool to the industrial problem.*





7. Can you provide relevant (validation) case studies to demonstrate the accuracy of your software in solving specific (industrial) problems?

SWO

If YES – please give an example. If NOT – please explain why.

- Case studies** published on web-page: 2
- Relevant scientific **publications, patents**: 3
- Benchmarks**, models and stories from **customers**: 2
- Tutorials**, general **descriptions** of models: 3
- Some case studies and validations are **confidential**: 3

How to stimulate the SWOs to provide non-confidential cases on certain industrial problems, demonstrating also the accuracy/limitations of their software?





8. Can you provide, if needed, special conditions/licences for SMEs to use your software? SWO

If YES – please give an example (that can be shared). If NOT – please explain why.

No: 7

3 licensing models:

Commercial
R&D
Academic

Yes: 3

Action for SWO and Translators:

➤ *Discuss procedures to provide special conditions/licences for SMEs*





9. Do you use/have other features of your model to profile it?

SWO

- I do not understand this question: 2
- No: 3
- Provide the scientific experience and develop the cooperation with university
- Data management plan
- Training company experts in modelling





10 -13 Questions

Questions 10-13:

There are only two persons who answers the questions. Unfortunately, both of them are not familiarly with the industrial use of materials modelling.

The companies use modelling not very intensive.

Criteria for choosing/using specific model/software:

Physics that need to be modelled

User friendliness

License costs

Time required to solve the problem

Good documentation

