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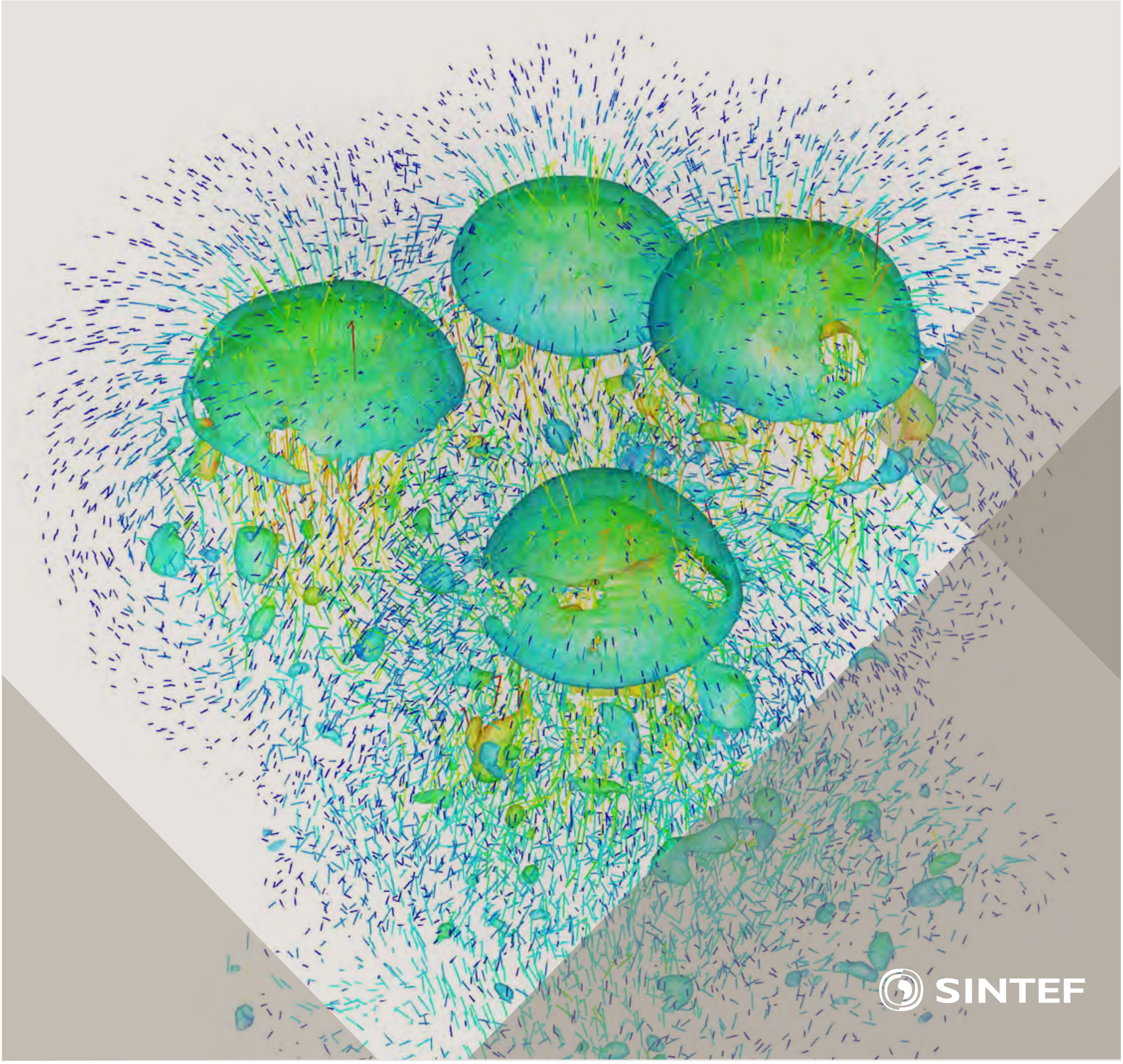
Selected papers from 10th International Conference on Computational Fluid Dynamics in the Oil & Gas, Metallurgical and Process Industries

Progress in Applied CFD



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Editors:
Jan Erik Olsen and Stein Tore Johansen

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PREFACE

This book contains selected papers from the 10th International Conference on Computational Fluid Dynamics in the Oil & Gas, Metallurgical and Process Industries. The conference was hosted by SINTEF in Trondheim in June 2014 and is also known as CFD2014 for short. The conference series was initiated by CSIRO and Phil Schwarz in 1997. So far the conference has been alternating between CSIRO in Melbourne and SINTEF in Trondheim. The conferences focus on the application of CFD in the oil and gas industries, metal production, mineral processing, power generation, chemicals and other process industries. The papers in the conference proceedings and this book demonstrate the current progress in applied CFD.

The conference papers undergo a review process involving two experts. Only papers accepted by the reviewers are presented in the conference proceedings. More than 100 papers were presented at the conference. Of these papers, 27 were chosen for this book and reviewed once more before being approved. These are well received papers fitting the scope of the book which has a slightly more focused scope than the conference. As many other good papers were presented at the conference, the interested reader is also encouraged to study the proceedings of the conference.

The organizing committee would like to thank everyone who has helped with paper review, those who promoted the conference and all authors who have submitted scientific contributions. We are also grateful for the support from the conference sponsors: FACE (the multiphase flow assurance centre), Total, ANSYS, CD-Adapco, Ascomp, Statoil and Elkem.

Stein Tore Johansen & Jan Erik Olsen

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10th International Conference on CFD in Oil & Gas, Metallurgical and Process Industries
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ON PRAGMATISM IN INDUSTRIAL MODELING

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ABSTRACT

Many natural or industrial processes are of extreme complexity, and where the time- and length scales range from an atomistic level to years and kilometers. Often the processes or phenomena consist of multiple sub processes in which each comprises its own length and time scales. An example can be production of aluminum by the Hall-Heroult process, where process streams or raw materials, flow dynamics and segregation in silos, with time varying quality, the feeding and operational routines, the reduction cells with numerous sub processes, and the tapping process, all make up a complete process. To optimize such production processes with respect to economic and environmental parameters we will have to develop models which can give the overall picture and at the same time be accurate enough to support the optimization process. As there are many dynamic aspects of an industrial production, the ultimate need will be a model which can compute much faster than real time and which can be used to support current operations and to develop new processes.

In this paper we discuss how this type of pragmatic industrial models can be developed. We will identify and discuss the tools needed for such an analyses, including the analyses process itself and the frameworks needed for such analyses. Key elements in our pragmatic modeling concepts are human knowledge, including capabilities to understand complex phenomena and how these can be modeled in a simplified but "good enough" manner, systematic use of existing information, systematic analyses of what information (model results) is needed and at which accuracy and speed the results must be produced. Another key element is the selection and collection of experimental data, organized and made accessible in an optimal manner to support the predictiveness of the pragmatic model. We propose that all types of data are organized by a "bridge" (modeling middleware) between complex scientific (aspect/phenomenon oriented) physical models, simplified models and process data. We believe that these types of pragmatic industrial models will enable a step change in both operation, operator training and process optimization, as well as design of new processes. Finally, in a case study, we apply our pragmatic modeling concept to the aluminum production process and discuss the implications of our proposed concept.

Keywords: Modeling, framework, pragmatism, industry, process.

INTRODUCTION

Position and Motivation

Many natural or industrial processes are of extreme complexity, and where the time and length scales range from an atomistic level to years and kilometers. Often the processes or phenomena consist of multiple sub processes in which each comprises its own length and time scales. An example can be production of aluminum by the Hall-Heroult process (Thonstad et al., 2001) where process streams or raw materials, flow dynamics and segregation in silos, with time varying quality, the feeding and operational routines, the reduction cells with numerous sub processes, and the tapping process, all make up a complete process. To optimize such production processes with respect to economic and environmental parameters we will have to develop models which can give the overall picture and at the same time be accurate enough to support the optimization process. As there are many dynamic aspects of an industrial production, the ultimate need will be a model which can compute much faster than real time and which can be used both to support current operations and to develop new processes.

It has been stated at a previous CFD conference in Melbourne that no metallurgical process has hitherto been designed based on CFD. At the same time significant CFD work has been done on metallurgical processes. Keeping in mind the extreme complexity in a full process we realize that CFD, applied to optimize a single process step without seeing this as element in a larger system, would not be capable of driving technological-economical step changes. We will therefore have to investigate ways to model a process; ways which are simplified, but fast and sufficiently accurate to serve its purpose. These models should be based on physics, which is critical to ensure predictive power. However, if these types of pragmatic industrial models can be developed, they will enable a step change in both operation, operator training and process optimization, as well as in the design of new processes.

Over many years SINTEF has been involved in research projects where the costumer's needs have been in focus and scientific excellence may conflict with the need to give the user something which can be applied immediately. Examples of this type of work are illustrated by following two applications:

1) Mitigation of large HF emissions in aluminum plants was studied by CFD. To run a larger parametric study the complex 3D problems were extremely simplified by smaller 2D problems. In this manner it was possible to complete the study and the results gave clear and, as later observed, successful advice.
2) In the second case (Johansen et al., 1998) melt refining of liquid aluminum was predicted and optimized with a simulation tool, which was based on a combination of 1D and 0D transient models, and where sub-scale information (closures) were obtained from experimental studies and 3D CFD simulations. With this approach it was possible to make sufficiently accurate predictions much faster than real time, allowing this to become an operational tool.

In general we have experienced that use of interpolation inside pre-calculated (by CFD or similar) tables is a powerful approach, to be used as part of a model or application. As an example we have made a complete application, which is based on interpolation within data obtained from CFD calculations. However, for design of the "experimental matrix" we see clear needs for scientific experiment planning methods, including high/low analyses and factorial designs, as crucial tools for generating such tables. These observations indicated the need for a more systematic and scientific approach in development of industrial models, and we need to start out from where the scientific community currently stands on these issues.

From scientific to pragmatic

The great efforts of the natural science community ensured that many phenomena can be understood to a high level of details. Of course, in many cases the existing techniques may have to be improved or new techniques developed, to obtain the required information. However, these detailed and accurate studies (numerical or experimental) usually require significant time. In many cases long-time work with detailed phenomena has resulted in engineering correlations such as wall friction in pipe flow. Hence, these correlations can be used to make very fast calculations of pressure drops and flow capacities. If we move to the more complex multiphase pipeline flows, development of accurate correlations becomes much more demanding, e.g. gas may flow as bubbles or a continuous fluid, while liquid flows as droplets and/or a continuous liquid. At the same time, droplets and bubbles are in continuous evolution due to coalescence, breakup, deposition and entrainment. Currently, we have direct simulation techniques that enable simulation of detailed bubbly flows (Lu and Tryggvason, 2007). Such simulations can be performed on volumes containing at most a few liters of fluid, and where the simulations over some seconds of real time may take several days on a high performance computer cluster. In an extreme industrial case like the potential Russian Shtokman pipeline, the volume of the flow line is around 10^{11} liters, and the flow time scales are of the order of weeks (10^6 sec). Accordingly, it is currently infeasible to simulate the transient flow in such a pipeline with a multidimensional approach. Our best hope is to develop simplified 1D models, which by learning from fundamental simulations, such as in Lu & Tryggvason 2007, and experiments, can be made accurate enough to be industrially useful. In the past, this has been done using different pragmatic approaches, although with varying success.

From pragmatic to scientific

As discussed above, we will in many situations need a pragmatic approach to obtain industrially relevant information. For the industrial user the model results must be available within a given time span. If not, the results may have no value. At the same time, the accuracy of the model should be quantified (probably a collaborative effort of the industrial user (case owner) and solution architects (see Figure 1 and Figure 2), such that the user knows the significance of the predicted results and recommendations. The industrial model will have to be built on different building blocks, which will have to be put into system (orchestrated) by a well-defined framework (our view on the elements of the pragmatic analysis and its analytical framework are illustrated in Figure 1). What emerges from this is a need to put all these critical elements into a scientifically founded framework. As has been learned from the past, not every pragmatic approach has been successful, urging that we need to put science into the pragmatism itself.

Structure of this work

This work is organized in the following way. The *Introductory section* of this paper gives our position and motivation for pragmatism in industrial modeling. We continue by discussing how to move from scientific analysis to its industrial counterpart, and vice versa. Both are important for effective and pragmatic contribution to the industry activities.

Section 2 takes a process view on pragmatic industrial analysis, including in addition to the modeling (a primary focus of our work) experimental activity, various theoretical analyses and organizational and management activities. Before focusing on modeling, it is important to enlighten its contribution to the total analytical process, and its interplay with other, equally important parts of the pragmatic analysis. This interplay of practical, holistically organized and orchestrated methods is the property that makes the pragmatic analysis so important for the industry and different from other scientific and research approaches.

Section 3 narrows our analysis on its modeling part. Our system view on modeling is inspired by software (SW) engineering. We start by discussing modeling frameworks (an effective way to organize modeling functionality and its SW realizations), existing research body and modeling industry trends. We continue by summarizing the research and scientific requirements for a modeling framework, and map them to SW engineering requirements. We suggest the necessary evolution of modeling frameworks, for their more effective industrial use. Thereafter we treat analysis and modeling as workflows, and give a simplified example of interacting models that are orchestrated and give solution/answer on an industry-relevant problem. This introduces section 4, which illustrates the modeling workflow on the example of industrial Al electrolysis.

Section 4 follows the analysis workflow logic suggested above on the example of industrial Al electrolysis (the Hall-Héroult process (Thonstad et al., 2001)). In this practical case the questions to be answered are:

- How does the heat loss from the process vary with the anode-cathode distance for the case when interfacial waves are neglected?
- What is the thickness of the frozen bath crust (side-ledge) as function of the anode-cathode distance?

Section 5 discusses our experiences with this theoretical and practical exercise and suggests future steps and improvements. We try to motivate the reader for future systematic treatment of the field "pragmatic industrial modeling", because the standardization and consolidation in industry and research, as well as SW technology, might lead to much more effective use and reuse of modeling, analyses and results.

For the reader's convenience we offer a list of terms and definitions at the end of the paper, because this multi-disciplinary paper uses many terms coming from SW engineering, system sciences and other research disciplines. We have tried to take over as much standard definitions as possible (from common Web definition sources (Web refs. 5, 9, 19, 20, 21, 23) , and slightly adjust them for our use. In such a way we want to contribute to the spirit of standardization of the research praxis, which this paper strongly advocates.

PROCESS VIEW ON PRAGMATIC INDUSTRIAL ANALYSIS

Pragmatic industrial analyses should be carefully organized, planned and executed. They require a structure not just in models, simulations, experiments, information and data, but also in analytical processes, concluding by well-structured communication of the results and the analytical context in which the results are valid. We see these important elements as parts of the analytical framework (FW), illustrated in Figure 1. Let us shortly discuss some of the important phases, and the results they produce:

1. ***Problem and Context Identification*** - this analytical phase requires discussions between the actors and stakeholders involved in industrial analysis. It includes clarifications of the use case, specification of the industrial/analytical context, agreement on needed accuracy of the solution, specification of necessary input and output information (its data formats etc.), as well as required interaction with other information systems and processes. Explicit simulations and experiments are agreed upon to answer given explicit questions. There are many SW Engineering tools, standards and methodologies available that can help structuring these important specifications (e.g. requirement analysis, use case specifications, pilot and demo exercises etc.). These analyses are grouped in ***step 1*** in Figure 1.
2. ***Analytical Strategy and Plan*** – Many industrial cases are complex and resource demanding and thus require a good analytical strategy and planning. This may be in contrast with the systems that will use their results (e.g. Decision Support Systems), because they might require information, which will be provided in real-time or nearly real-time conditions. Thus, in some cases, it will not be possible to give the answer with sufficient speed and accuracy. In such cases we need to carefully plan the experimental work or numerical experiments. Correct analytical strategy and planning (e.g. including metamodeling techniques) is critical for obtaining the results, which can be properly analyzed and qualified (illustrated as ***step 2*** in Figure 1). Several statistical methods, such as Analysis of variance (ANOVA), are available to analyze how combinations of input parameters may impact the results. Example tools that support executing such analyses are DAKOTA (Web ref. 8) and Mode Frontier (Web ref. 15).
3. ***Architecture of the Analytical Framework*** - The agreed analytical questions will often need models at many different levels to give acceptable answers. As the complexity of a model increases, the organization of the models will require a framework for systemizing and orchestrating its sub models. Such an analytical framework must

be well structured, applying an organized set of models, simulations, experiments and related information/data structures (***step 3*** in Figure 1). An example of such a framework is the volume-averaging technique (Whitaker, 1969 and Soo, 1989). The volume-averaging technique allows the derivation of continuum based conservation equations, based on a continuum model for the underlying materials and fluids. The approach allows multiple layers of averaging, which allows treatment of very complex systems. Such a procedure is also known as multi-scale or multi-level modeling (Ghosh, 2011).

4. ***Execution (Orchestration of Analyses, Simulations and Experiments)*** – by completing the first 3 steps illustrated in Figure 1, the necessary set of models, simulations, experiments and other analytical procedures are prepared, and one can proceed with the ***step 4***, - orchestrating them in a holistic analysis. Such an orchestration might include various modeling and analytical techniques, varying in complexity and heterogeneity, e.g. meta-modeling becomes increasingly important as the complexity of models increases. In the case of multilevel modeling, the volume averaging techniques are critical in analyzing, constructing and developing part of the model framework. The volume averaging technique, when applied to a class of problems, will allow reuse of models, rules and constraints. When the analysis of the problem indicates that the time required to answer a request from a higher level in the model hierarchy is too great, we have to resort to pre-calculations or experiments. This is fully possible if a robust procedure for this is developed.
5. ***Evaluation of the Solution*** - When we are doing experiments or simulations to answer posed questions, it is critical to understand the consequence of modeling results. It is tempting to make one prediction and give a fast feedback. However, we need to have a systematic approach to assessing the results (***step 5*** in Figure 1 – solution analysis). From experience, it is well known that simulation models have many weaknesses, as well as the human limited knowledge. This imperfection is illustrated by giving 10 different, but qualified people, an industrial problem and asking for the solution based on a given code (common to them all). This can result in 10 different answers, owing to differences in understanding of the problem and what it takes to solve the problem. An obvious deficiency is the lack of standards for problem definition, requirements to the accuracy of the results, communication, and interpretation of input and output data. Such challenges illustrate that our systematic approach must try to reduce the uncertainty in predictions and for now primarily by quantifying it. Then we have obvious reasons to apply ANOVA methods on both numerical and experimental data, as well as their combinations. Hence, it will be possible to quantify the accuracy of a given answer to a given question. The knowledge extraction process will often require handling of large data sets or streams. In these cases the productivity will be increased by using script based analysis tools such as MatLab (Web ref. 14) or Octave (Web ref. 16).
6. ***Conclusion and Communication –*** it is very important to conclude pragmatic analysis by a communication of the analytical results (step 6 in Figure 1). Usefulness of produced and published modeling and analytical results is often limited, because it is not well related to the analytical context. It is important to relate the analysis to its context, containing among others: (a) important analytical parameters, (b) information about modeling scale, (c) accuracy of the proposed solution, (d) estimates of representability, (e) predictive power, (f) computing and experimental resource consumption, etc.

   Information about analytical context is needed not only for the evaluation of existing models/analyses/experiments, but also for their future use and reuse. One could even require that such information is standardized, and in such a way facilitate efficient and standard interworking (and possibility to combine existing and new analyses in solution of industrial problems).

If we succeed in standardizing, we might even manage to "decouple" the analyses from their context and reuse them in new applicable analytical situations (context). One of the reasons why a given model is not used widely is that it may suffer from lack of analytical transparency.

In the engineering literature there are no clear strategies for how a complex model should be designed, assembled and qualified. Most typical is to build the model based on some specification, or let the model develop organically. However, industrial models very often have clear specification of the needed time response, accuracy, formats for information flow, as well as the rules and the framework for building the entire model system (frequently specified by requirements and/or use cases). To give one example:

The accurate prediction of liquid holdup and pressure drop in multiphase pipelines is of significant industrial value. A 3D model takes typically two orders longer time than a 2D/Q3D model, which typically takes two orders longer time than a 1D flow model. These models are extremely time-consuming compared to a multiphase point model (steady state) which typically can produce results in 1 ms or faster. Still, even such an efficient model has around 15 input parameters (properties, geometry, and velocities). If we want to cover a full matrix with 10 values for each input parameter, simulation of the matrix once will need more than 18 years of CPU time. This illustrates that we need a scientific approach to all phases of pragmatic industrial modelling, and standardization and systematization of its phases.

SYSTEM VIEW ON INDUSTRIAL ANALYSIS - MODELING FRAMEWORKS

This section focuses on the modeling part of pragmatic industrial analysis (phase 3 and 4 in Figure 1). Our system view on modeling is inspired by SW engineering. We start by discussing requirements for modeling frameworks, comment on existing engineering efforts, research and industry trends. We suggest standardization and development actions for modeling frameworks, which will enhance their effective scientific and industry use. We also analyze the modeling with help of scenario and workflow techniques and give a simplified example that will be used in the practical example in section 4.

Existing research and engineering work

Based on observations from industrially related development work over many years (some referenced below), we see that there is a need for a well-structured, scientifically founded, and highly standardized framework for developing industrial models. Such a framework should be well defined in several perspectives: e.g. domain knowledge (e.g. physics, chemistry, structural mechanics…), mathematical/numerical aspects, and SW engineering perspective.

In this section we discuss the SW engineering perspective, which focus on the modeling frameworks (often called modeling platforms), their modeling elements/modules, and their architecture, topology and implementation technology.

The main purpose of so-called "pragmatic modeling" is to adjust the research models to the realism/world of industrial processes, their scope, perspective and challenges. So-called industrial models have requirements as: (a) industrial scope and perspective, (b) usefulness, (c) required accuracy and predictiveness, (d) simplicity of use, (e) response time and speed, (f) compatibility with other (industrial) models, etc.

To meet the above-mentioned requirements, the number of the "practical" system and SW engineering requirements have to be realized, e.g.:

- Interactivity with well-established industrial standards,
- Modularity,
- Clear interfaces / API with other models and modeling tool-boxes,
- Compliancy with industrial and SW engineering standards,
- Well-defined "insertion procedures" and interaction rules in calculations (meshing interactions, initial and boundary condition inclusion, libraries of user-defined functions, procedures for solver algorithms changes etc.),
- Inter-model interworking and interoperability,
- Well-structured and standardized raw data and metadata,
- Documentation.

There is currently extensive work on modeling technology, showing variety of approaches, modelling architectures, modeling strategies, modeling technologies, e.g. expert systems based on qualitative reasoning engines and elements of AI (Enemark-Rasmussen et al., 2012), hybrid multi-zonal CFD models (Bezzo et al. 2004), coupling modeling and decision tools (Rossig et al., 2010), model-centric support for manufacturing operations (Rolandi and Romagnoli (2010)), and optimizations by reduced CFD models (Lang et al., 2011).

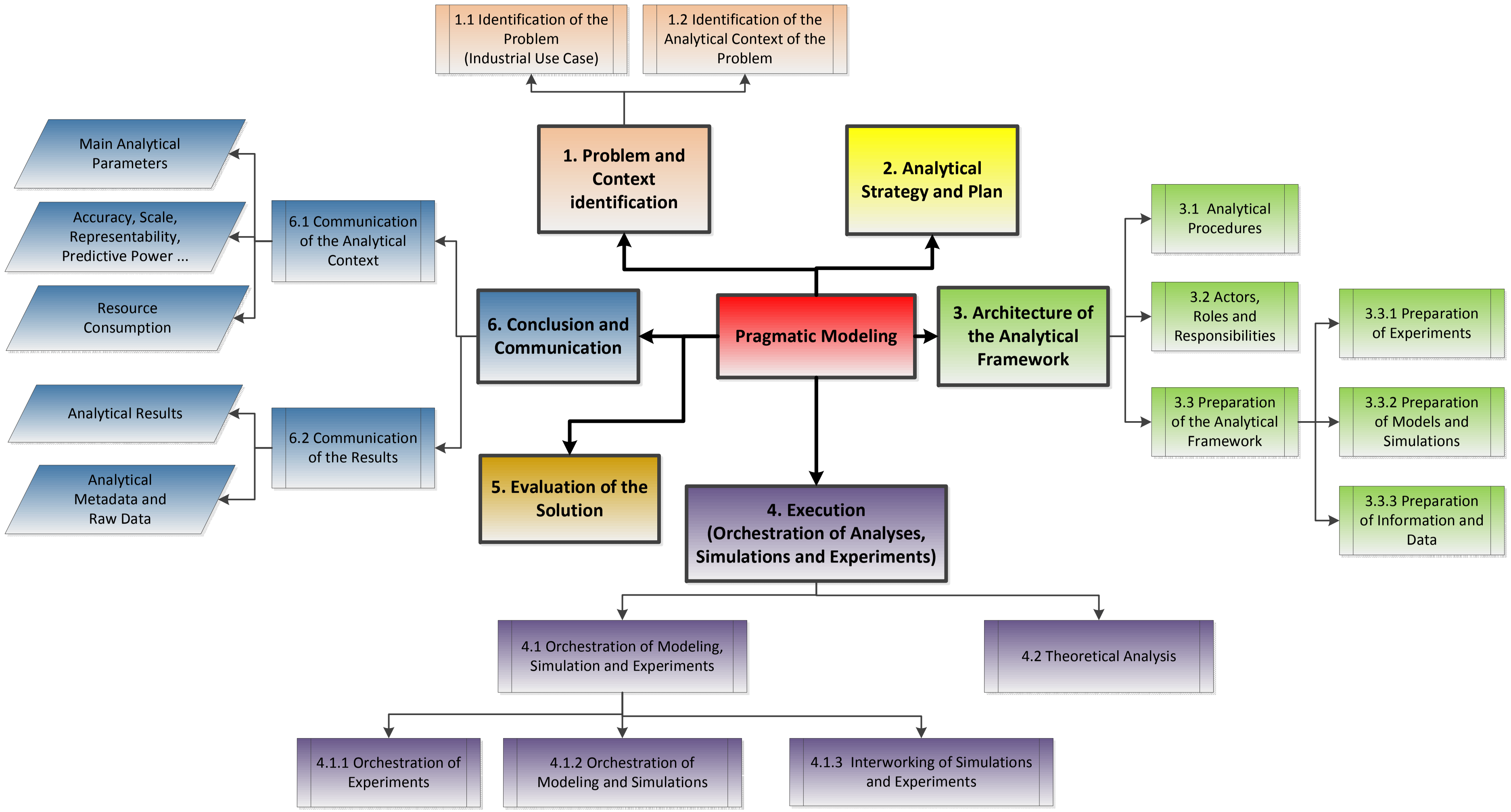


Figure 1. Some of the important phases, processes and results in a typical pragmatic analysis (terms and definitions are given in section 1).

Various model types are being combined in solutions of industrial problems, e.g.: (Rolandi and Romagnoli, 2010), (Chen, 2001), (Malawaki et al, 2005), (Power and Sharda, 2007), Urban et al. 2009). CFD models are used for different purposes. Power and Sharda (2007) discusses embedded quantitative models in Decision Support Systems. Authors emphasize that the nature of interconnected models can vary from algebraic, decision analytic, financial, simulation, optimization and many other types. Power and Sharda (2007) stresses the need for standardization of data structures (XML), protocols and other involved ICT technologies. Lang et al., 2011 discusses the need for standardization of industrial models, with example of computer-aided process engineering (CAPE). Authors emphasize two particular advances the industry can benefit from: (1) general-purpose custom-modeling platforms and (2) standardization of interface specification for component-based process simulations.

Rolandi & Romagnoli 2010, as well as Urban et al. (2009) stress the lack of development of both high-level frameworks and low-level mechanisms to assist the formulation of "models" of process engineering problems for support of process operations.

Rolandi & Romagnoli 2010 divides the framework models in several categories: (a) first-principles process models, (b) high-fidelity process models, (c) plant-wide process models, (d) large-scale process models. They also discusses different modeling framework components, used in various phases of the modeling/analytical process: the data pre-processing environment, the estimation / reconciliation environment, the consistent data etc. They give a schema for typical modeling activities included in a typical framework for integrated model-centric support of process operations.

Lang et al., 2011 describes a use of reduced order CFD models in optimization of IGCC processes. The procedure for development of reduced order models (ROM) is explained in Lang et al., 2011 and Lang et al. 2009. They "wrap" the ROM to fit the modular framework of the simulator. Lang et al., 2011, expects that the future work will continue the improvement of methods to develop accurate and efficient ROMs from CFD models, along with their integration and validation within process optimization environments.

This implementation will also be extended to the CAPE-OPEN software standard (Web ref. 6) and to integration within the APECS system.

Several industrial initiatives (Web ref. 12) and open standards / approaches, such as in (Web ref. 6), are getting momentum; however, at the current time, generic, standardized frameworks for scientific computing are not wide-spread. Several software vendors are instead progressing towards product-centric multiphysics frameworks, such as ANSYS workbench (Web ref. 1) and COMSOL Multiphysics (Web ref. 7). However, a two way connectivity of such software platforms, such as recently realized between MATLAB (Web ref. 14) and MAPLE (Web ref. 13), has still not been fully realized.

Industry makes efforts towards proprietary customizable workbench solutions, which enable connecting external tools to their solutions. Workbench solutions include a combination of standard scripting languages, e.g. Python (Web ref. 1), data standards and interfaces, standardized modeling techniques, with well-defined protocols (Web ref. 1 and Web ref. 2). Such tools combine technologies as: bidirectional CAD connectivity, powerful highly-automated meshing, project-level update mechanisms, pervasive parameter management and various integrated optimization tools. Examples of these customizable modelling technologies include references (Web ref. 6, 8 10, 15, 17, 18).

Several strategies (both centralized and decentralized modeling approaches) to "bridging" scientific and industrial models are used in praxis:

- **Direct inclusion** of new scientific models (or their approximations / simplifications) into industrial models – enrichment of industrial models, (e.g. via libraries of user-defined functions, modification in calculation procedures / algorithms, new modeling modules, new solvers etc.)
- **Building completely new industrial models** – from scratch, based on the newest achievements of scientific models and equation solver strategies.
- **Orchestration** of various model types (e.g. script-based orchestration of models with well-arranged information exchange between models). A combination of extra-model orchestration (middleware-based) and intra-model interventions (by changing user-defined functions (UDFs), boundary conditions etc.), exchange of input/output files etc.

We expect that the future evolution of modeling frameworks for pragmatic modeling will (with respect to the topology) head in two directions:

(1) *Centralized architectures* (main modeling tool controls the modeling/simulation process, including underlying tools and modeling elements) and

(2) *Decentralized architecture*s (middleware for model orchestration: script-based or middleware-based orchestration of various models and modeling tools).

We would like to motivate further development and standardization of the SW engineering related to modeling frameworks, e.g.:

- **Standardization of the modelling middleware including standardization of:**
    - Application Programming Interfaces (APIs) and protocols, and their module-like implementations,

  - Scripts for orchestration of models, and related workflow like data exchange,
  - Monitoring, logging and control routines and mechanisms.
- **Standardization of data exchange formats (e.g. XML-based)...**
- **Standardization of modelling metadata:**
  - Specifying the analytical context in which industrial problem will be solved.
  - Specifying the accuracy, sensitivity and quality of models and simulations (this can be organized as a part of the analytical context).
  - Ensuring the description of the data entities, models, their modules and processes.

Modeling workflow – a scenario perspective

Pragmatic modeling is often a part of a complex analytical and/or design process (Figure 1). It is a team work, as illustrated by Figure 2, driven by analytical workflows (often structured by usage/analytical scenarios (Figure 2- Figure 4)). It employs a modeling framework / architecture and a set of modeling technologies. The system architects specify a set of data/information exchange standards, protocols and interfaces (to mention just a few SW design artefacts), a number of design tools (e.g. Web ref. 8 and 15) and modeling tools (Web ref. 3 and 14). Designers and analytics verify often the results by various model analyses and fine-tuning techniques (e.g. sensitivity analyses – evaluated against physical elements).

Figure 2 gives a high-level over-simplified illustration of an abstract analysis/design process, which will include modeling support in its decision-making. It illustrates pragmatic modeling roles and scenarios, modelled in unified modeling language (Web ref. 22).

Figure 3 shows the main analysis process as a Sequence Diagram (Web ref. 22). Main Analysis triggers the Analysis 1, the algorithm of which relies upon the Analyses 2 and 3. The interaction of various analyses and their respective models is shown as sequence diagram interactions. One interaction can involve several data/information exchange processes and respective algorithms.

Figure 4 details the interaction between the Analysis 1 and the Analysis 2 (illustrated in Figure 3). In this figure we see the details of the algorithm of the Analysis 2 and the data/information exchanged among its model elements.

These high level diagrams (Figure 2- Figure 4) illustrate the SW engineering view on modeling. We will illustrate it by concrete examples offered in Section 4. We use SW-focused view to discuss the requirements and SW Engineering issues related to model interaction, data/information exchange, interfacing, standardization and other important elements for design of pragmatic models.

PRACTICAL EXAMPLE

Analysis 1 – Aluminum electrolysis

Primary aluminum is manufactured exclusively by the Hall-Héroult process (Thonstad et al., 2001). The process is based on electrolytic decomposition of alumina dissolved in a fluoride mixture serving as electrolyte at 960 ^{o}C, using consumable carbon anodes and horizontal anode configuration. A cross-sectional view through a typical electrolysis cell is shown in Figure 5).

Owing to the high temperature, highly corrosive and opaque environment, the interior of the cell has limited access for inspection and measurement, and the processes taking place are strongly coupled. It is, therefore, necessary to apply models for predicting how the entire system will react on changes in construction or operation. For instance, to optimize the energy consumption in the cell, such changes could be related to the anode topology,

In the Hall-Héroult process, several questions may be asked, which need to be answered by models and modeling frameworks. In the present example the main question to be answered is:

- How does the heat loss from the process vary with the anode-cathode distance for the case when interfacial waves are neglected?
- Additional response requested: What is the thickness of the frozen bath crust (side-ledge) as function of the anode-cathode distance.
- Answering such questions requires some mathematical model, as direct empiric is insufficient for such an extremely complex process. As a result of the complexity and requirements to get fast and at least qualitatively correct answers, a large number of partial process models have been developed in Microsoft Excel (Web ref. 11). Such models are for instance used for predicting the current efficiency, the cell voltage, the energy balances taking into account the enthalpies for the main chemical and electrochemical reactions as well as the distribution of the heat losses, and finally the temperature, pressure, and gas composition inside the cell superstructure and the flue gas scrubbing system. All partial models are based on first principles wherever possible and include fitted experimental and numerical data.
- Considering our posed question above on the overall heat loss, we simplify the heat loss from the central part of the cell bottom by regarding this as a 1D problem, and calculating the heat loss by standard engineering formulas for a layered structure. The heat loss from the sides and ends are calculated by subdivision of these regions into a number of 2D elements connected by thermal resistances depending on the cell geometry and the thermal conductivities of the materials used.

The heat loss through the different parts of the top of the cell (crust, anode, anode stubs) is computed by analytical expressions derived from numerical calculations and real measurements. The cell voltage is based on similar approaches, ranging from standard engineering formulas (ohmic resistances) via thermodynamic and electrochemical data (reversible cell voltage) to fitted laboratory and numerical data (overvoltages).

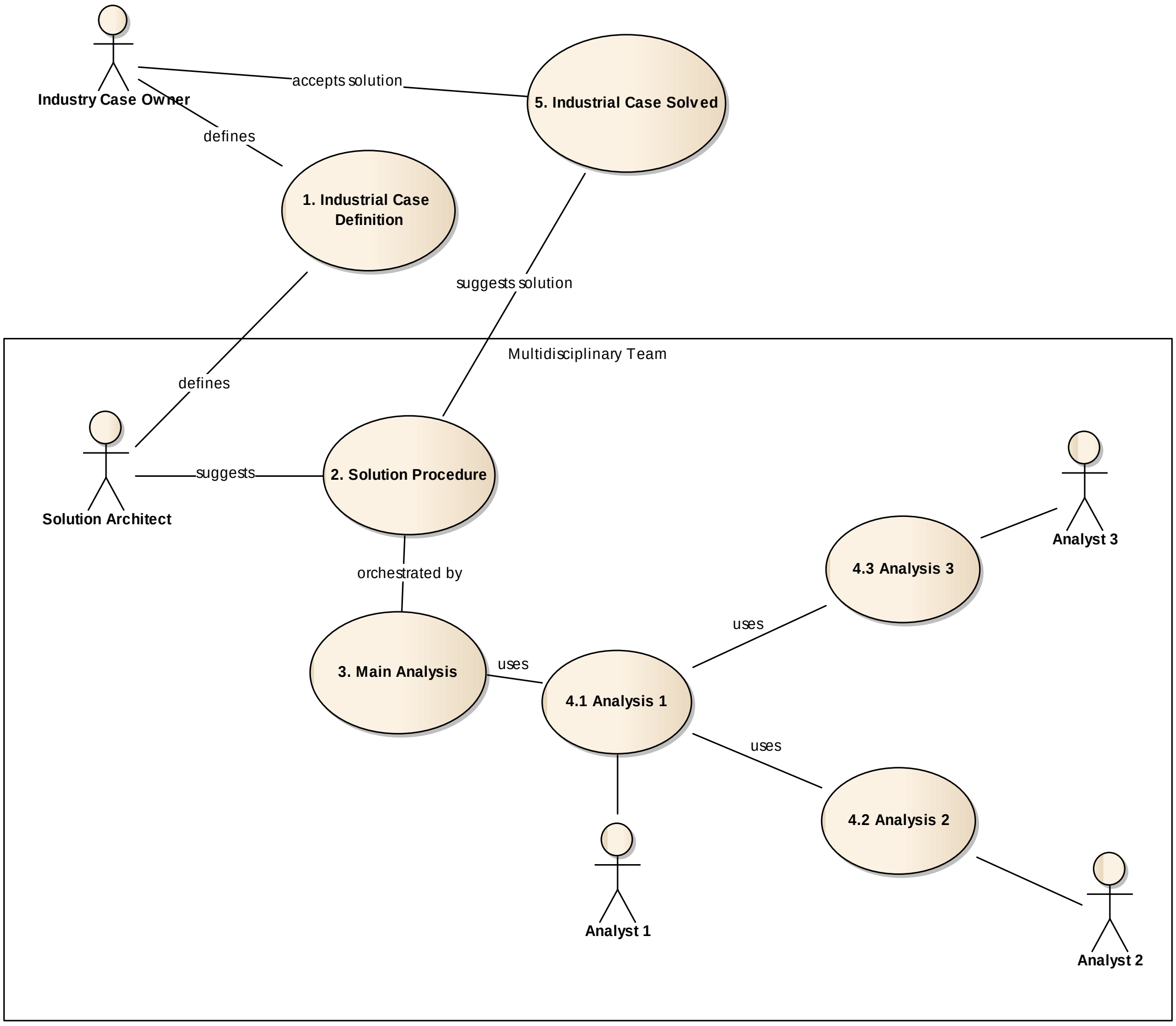


Figure 2. Use case diagram (modelled in Unified Modeling Language (Web ref. 22)). illustrating a simplified collaboration among actors (with their roles and responsibilities) in a pragmatic industrial modeling process.

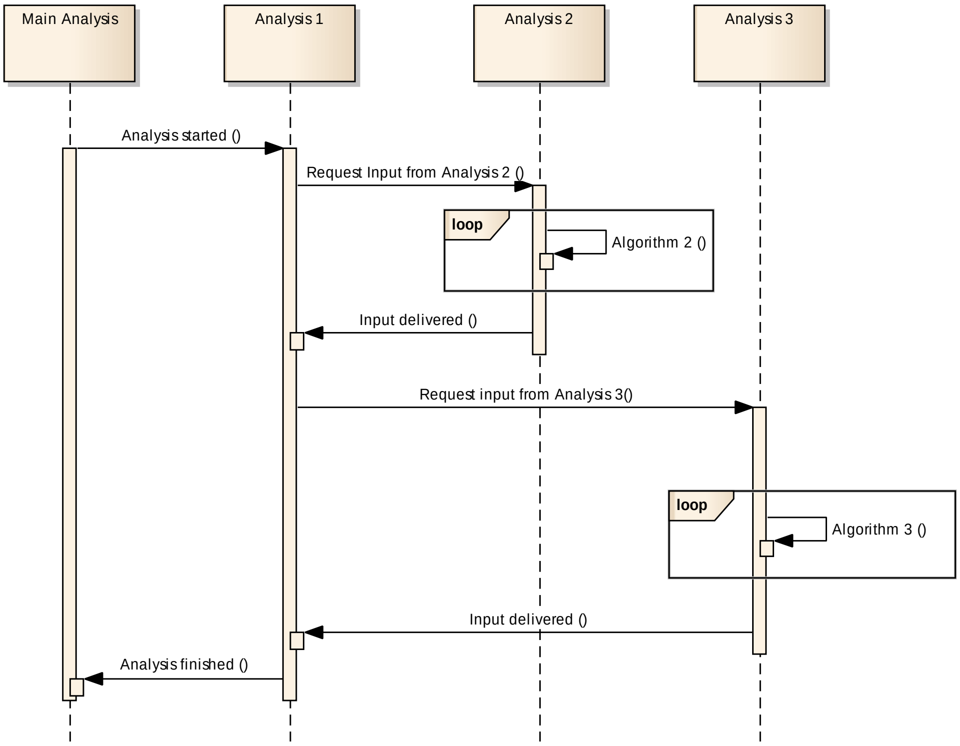


Figure 3. Sequence diagram (in Unified Modeling Language (Web ref. 22)) illustrating the partial realization of the use cases for the Main Analysis (shown in Figure 2).

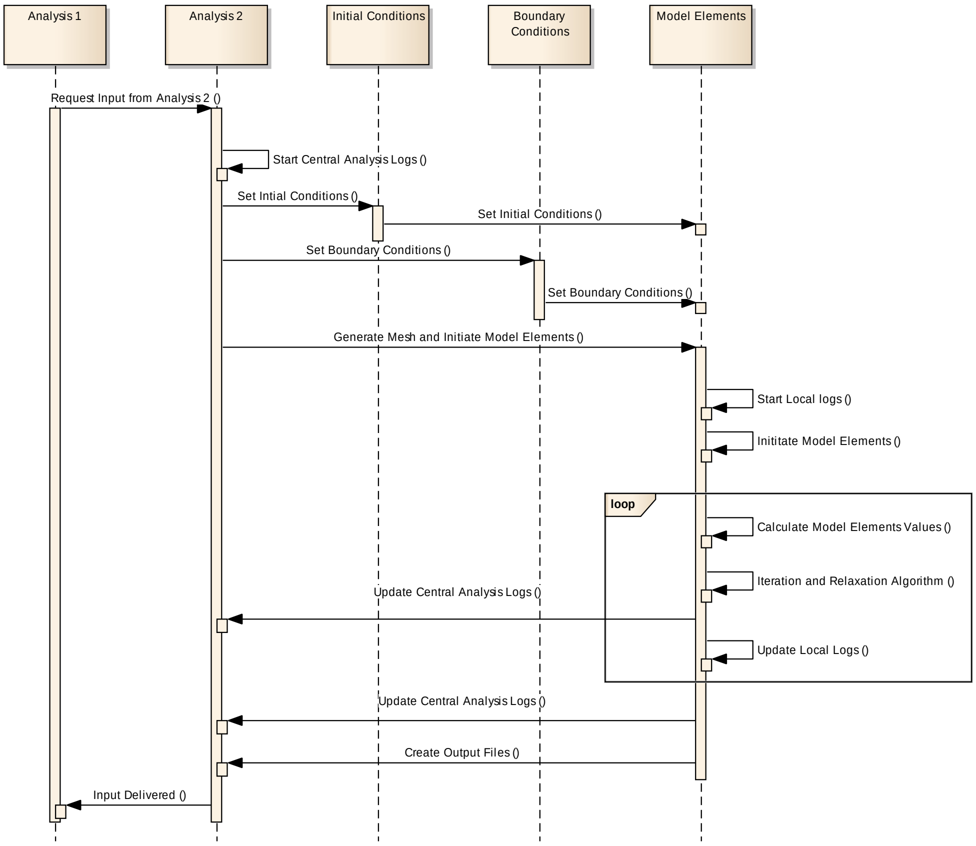
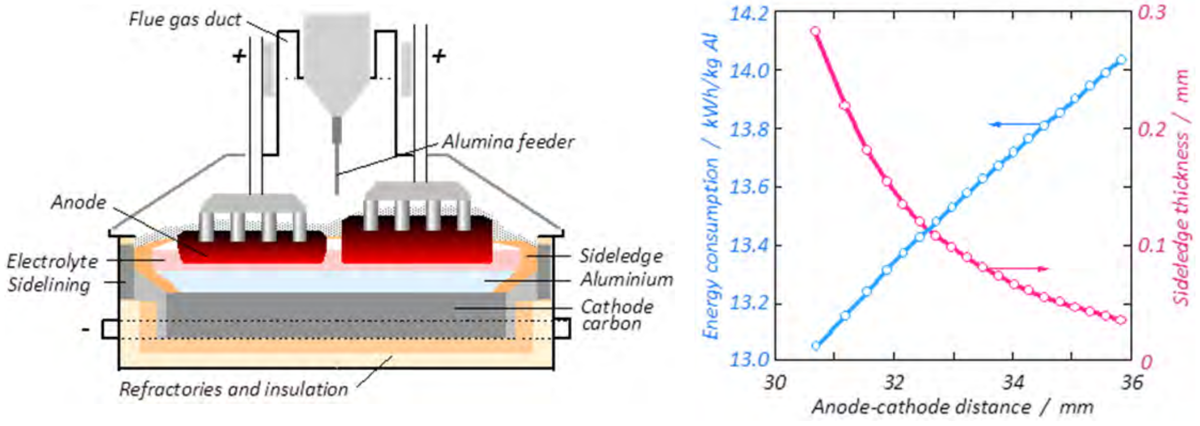


Figure 4. Sequence diagram detailing the realization of the use case "Analysis 2" from Figure 3.



a) *b)*

Figure 5. ***a)*** Schematic cross-section through an aluminum electrolysis cell, ***b)*** Predicted energy consumption and side ledge thickness versus anode-cathode distance.

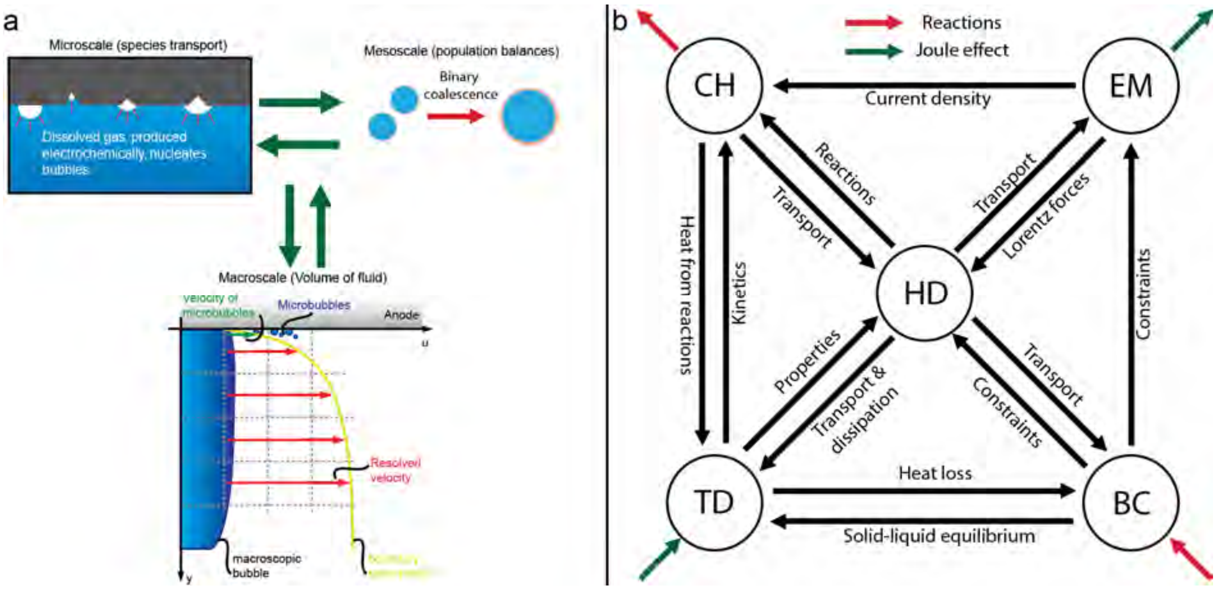


Figure 6. Schematic of multiscale approach a), and principal coupling diagram b), indicating the coupling between different phenomena in an electrolysis cell; chemical reactions (CH), electromagnetism (EM), boundary conditions (BC), thermodynamics (TD) and hydrodynamics (HD).

Some of the partial models can be used as stand-alone models, but they are all included in a total electrolysis cell modelling framework, allowing for coupled calculations and thus a holistic understanding of the overall heat balance of the cell.

The main numerical task in the framework is related to adjusting the anode-cathode distance of each individual anode until the cell voltage and the total current equal the pre-determined values, and the thickness of the side-ledge is varied until the total heat loss exactly balances the difference between the total energy input and the change in enthalpy in the process. Unfortunately, there is no way of measuring the anode-cathode distance accurately, and this parameter must be calculated from the bath voltage. The bath voltage is the difference between the total cell voltage and the remaining voltage terms, which can be either measured or modelled. The electrochemical overvoltage and the extra voltage drop due to the shielding effect of the gas bubbles ("bubble overvoltage"), which both are significant, are however difficult to measure. Presently, the calculation of the "bubble overvoltage" is based on a water model. Today, it is within reach to use CFD modelling to obtain better data on the extra resistance due to bubble shielding resulting from different complicated anode geometries , and being a function of the gas evolution rate and flow conditions. As response to the questions posed above, a typical answer (prediction) from the model is seen in Figure 5b).

If the required correlations for bubble overvoltage are not available for the current configuration, for instance due to a novel anode design, the current analysis will ask for specific input (for instance a correlation between bubble overvoltage, anode topology and current density) from an analysis performed by a separate model framework. The calculation of such a correlation is exemplified in the following section.

Analysis 2 – Gas Evolution in Al Electrolysis

A simulation framework allowing for the description of bubble evolution on a single anode has recently been developed (Einarsrud, 2012), based on a multiscale coupled population balance / Volume of Fluid approach, as sketched in Figure 6 a): On a (micro) species level, gas is produced electrochemically by the presence of an electrical current. Following saturation, mesoscale bubbles are formed, treated by population balance modeling. As small bubbles evolve due to coalescence and mass transfer, macro-scale bubbles are formed, treated by the Volume of Fluid method. Owing to low electrical conductivity, the presence of bubbles alters the current density, consequently altering the distribution of gas on the microlevel, and thus also future nucleation events. Evidently, such a framework involves coupled phenomena spanning several disciplines, as indicated in Figure 6 b).

The *simulation* framework is fully orchestrated within the user-defined-function (UDF) functionality available in ANSYS FLUENT (Web ref. 3), allowing a user to add and couple additional models to the solver, based on specific macros supplied by the solver. The execution order of the conservation equations (i.e. mass, momentum, turbulence and scalar fields) is fixed by the solver, while the additional required UDFs can be executed either following each iteration or each time step. Currently, resulting source terms, for instance Lorentz forces, are calculated based on converged values of the fields at the previous time step, i.e. a time-splitting scheme is adopted. As the UDFs can be used to specify only specific terms used (although choices are vast) and that the overall execution order is dictated by the solver, this is an example of a product specific orchestration.

Considering the calculation of bubble induced voltage drop, several values must be given initially, for instance the nominal current density, system temperature, fluid properties and sought anode position in the cell, all of which can be supplied from the main analysis described above. Moreover, the anode shape and surface structure (i.e. porosity distribution) are required for realistic simulations. These properties can be obtained by other modelling approaches or material databases. The conditions supplied from other models and databases serve as initial and boundary conditions for the bubble flow simulation, as sketched in Figure 6 for a general analysis.

Following meshing, on a coarse or fine level, depending upon sought accuracy and time constraints set by Analysis 1, and initialization, the bubble simulation loop is initiated and run following a specific order, based on source terms and material properties obtained at the previous time step:

1) Flow, mass and turbulence equations are solved.
2) Electrical potential is solved, and current densities are determined.
3) Additional scalar fields are solved, representing chemical species and bubble number densities (population balance model)
4) New source terms are calculated based on converged fields, initiating the next time step.

After reaching a statistically steady state, the bubble induced voltage component is monitored and averaged for a given amount of time, finally yielding the output sought by Analysis 1, which in this specific example is a correlation between bubble overvoltage, anode topology, current density and electrolyte composition. This correlation can now be returned to the model in Chapter 4.1, yielding the required output, using the requested data format.

Our experiences with this practical modeling exercise (where we have tried to follow the modeling and analytical framework mindset (section 0)) show that significant energy has been used to establish a common view on the problem, understanding of the analytical context, the common knowledge base and the common problem dictionary. When those obstacles have been removed, the orchestration of various analyses towards the final solution was reduced to a manageable problem.

With respect to SW engineering technology, our modeling FW was based on a combination of "in-house" developed models (Excel (Web ref. 11) – based macro development (Analysis 1), with a customized workbench solution – based on ANSYS FLUENT product portfolio (Web ref. 1 and 3). We preferred to work as close as possible to industry standards, and the closest available approach was the customization of the widely-accepted SW products.

With respect to standardized processes for pragmatic industrial analyzes we have not found available and wide-spread methodologies. Therefore we have proposed the approach illustrated in Figure 1 and described in sections 2 and 3.

DISCUSSION AND CONCLUSION

In many situations a pragmatic analytical and modeling approach is needed to obtain industrially relevant information. For the industrial user the model result should be available within a given time span. If not, the results may have no value. At the same time, the accuracy of the model should be quantified, such that the user knows the significance of the predicted results and resulting recommendations. The industrial model will have to be built on different building blocks, which will have to be put into system (orchestrated) by a well-defined analytical and modeling framework.

Our view on the elements of the pragmatic analysis and its analytical framework is illustrated in Figure 1. What emerges from this is a need to put all these critical elements into a scientifically founded framework. As has been learned from the past, not every pragmatic approach has been successful, urging that we need to put science into the pragmatism itself. We believe that all of the six phases in a typical industrial (pragmatic) analytical process illustrated in Figure 1 can be to some extent standardized, e.g.: (1) problem and context identification, (2) standardized strategy and planning, (3) architecture of the analytical framework, (4) standardized orchestration and execution, (5) standard ways and criteria to evaluate the solution, and (6) standards for communicating the results and analytical context (for which they are valid, and usable). We can standardize the structure of the processes, the tools that are used, the quality assurance methods, as well as establish standards for how the results and analytical context are presented and described.

We would like to motivate the establishment of a scientific discipline that will focus on pragmatic industrial analyses and modeling frameworks. The effort of transforming the scientific results to industrial praxis is not just a methodological approach, but also a strategic activity. We hope that this paper and our technical opinion will contribute to establishing such a knowledge body.

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Web ref. 2: ANSYS DesignXplorer®, http://www.ansys.com/Products/Workflow+Technology/ANSYS+Workbench+Platform/ANSYS+DesignXplorer

Web ref. 3: Ansys, Fluent, http://www.ansys.com/Products/Simulation+Technology/Fluid+Dynamics/Fluid+Dynamics+Products/ANSYS+Fluent

Web ref. 4: Aspen Custom Modeler, https://www.aspentech.com/products/aspen-custom-modeler.aspx

Web ref. 5: http://www.businessdictionary.com/definition/

Web ref. 6: The CAPE-OPEN Laboratories Network, www.colan.org.

Web ref. 7: COMSOL Mulitiphysics, http://www.comsol.com

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Web ref. 9: http://www.dictionary.reference.com

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1. TERMS AND DEFINITIONS

Table 1. List of terms and definitions.

(To offer as standard approach as possible (with respect to industry, SW engineering and usual modeling and simulation praxis), all the definitions in the paper are taken over from the common Web definition sources (Web ref. 5, 9, 19, 20, 21, 23) and sometimes slightly adjusted for the use in this paper.)

Term	Definition (Definitions are taken over from the following Web definition sources - references (Web ref. 5, 9, 19, 20, 21, 23), and sometimes slightly adjusted for the use in this paper.)
Analytical Process	• A method of studying the nature of something or of determining its essential features and their relations (Web ref. 9). • In this work – a chosen method for studying an industrial problem, containing a number of well-defined steps, and results, with clear roles and responsibilities for participating actors (see also FIGURE 2).
Framework (FW)	• A skeletal structure designed to support or enclose something (Web ref. 9). A frame or structure composed of parts fitted together (Web ref. 21), the manner of construction of something and the arrangement of its parts (Web ref. 21). The underlying structure; "providing a factual framework for future research" (Web ref. 21). • In general, a framework is a real or conceptual structure intended to serve as a support or guide for the building of something that expands the structure into something useful (Web ref. 19). • In computer systems, (definition used in Web ref. 19) a framework is often a layered structure indicating what kind of programs can or should be built and how they would interrelate. Some computer system frameworks also include actual programs, specify programming interfaces, or offer programming tools for using the frameworks. A framework may be for a set of functions within a system and how they interrelate; the layers of an operating system; the layers of an application subsystem; how communication should be standardized at some level of a network; and so forth. A framework is generally more comprehensive than a protocol and more prescriptive than a structure (Web ref. 19). • In this work – we will mostly use the definition taken from computer system sciences (Web ref. 19).
Analytical FW	• In this work – a conceptual structure of various analytical methods (experiments, modeling, simulations, theoretical analyses), incorporated and orchestrated in an analytical process.
Modeling FW	• In this work – we take over the definition taken from computer system sciences (Web ref. 19), and use it in modeling, simulations and related SW engineering activities.
Orchestration	• Orchestration describes the automated arrangement, coordination, and management of complex computer systems, middleware, and services (Web ref. 23). • In this work we discuss orchestration of modeling, simulation and analytical processes in general.
Unified Modeling Language (UML)	• The Unified Modeling Language (UML) is a general-purpose modeling language in the field of software engineering. The basic level provides a set of graphic notation techniques to create visual models of object-oriented software-intensive systems. Higher levels cover process-oriented views of a system (Web ref. 22 and 23).
Use Case	• In software and systems engineering, a use case is a list of steps, typically defining interactions between a role (known in UML as an "actor") and a system, to achieve a goal. The actor can be a human or an external system. In systems engineering, use cases are used at a higher level than within software engineering, often representing missions or stakeholder goals (Web ref. 22 and 23).
Scenario	• A predicted or postulated sequence of possible events (Web ref. 21), an outline of the plot of dramatic work, giving particulars of the scenes, characters etc. (Web ref. 21). (We can talk of modeling scenarios, simulation scenarios, usage scenarios, analytical scenarios etc.)
Workflow	• The set of relationships between all the activities in a project, from start to finish. Activities are related by different types of trigger relation. Activities may be triggered by external events or by other activities (Web ref. 9).
Sequence Diagram	• A sequence diagram is an interaction diagram that shows how processes operate with one another and in what order. A sequence diagram shows object interactions arranged in time sequence. It depicts the objects and classes involved in the scenario and the sequence of messages exchanged between the objects needed to carry out the functionality of the scenario. Sequence diagrams are typically associated with use case realizations in the Logical View of the system under development (Web ref. 22 and 23).

Interface	• In computer science, an interface is the point of interaction with software, or computer hardware. Some computer interfaces can send and receive data, while others can only send data (Web ref. 23). The types of access that interfaces provide between software components can include: constants, data types, types of procedures, exception specifications and method signatures (Web ref. 23). The interface of a software module is deliberately kept separate from the implementation of that module. The latter contains the actual code of the procedures and methods described in the interface, as well as other "private" variables, procedures, etc. (Web ref. 23).
Application Programing Interface (API)	• In computer programming, an application programming interface (API) specifies how some software components should interact with each other (Web ref. 23). An API specification can take many forms, including an International Standard such as POSIX, vendor documentation such as the Microsoft Windows API, the libraries of a programming language, e.g., Standard Template Library in C++ or Java API. Web APIs are also a vital component of today's web fabric. An API differs from an application binary interface (ABI) in that an API is source code based while an ABI is a binary interface (Web ref. 23).
Middleware	• In the computer industry, middleware is a general term for any programming that serves to "glue together" or mediate between two separate and often already existing programs. A common application of middleware is to allow programs written for access to a particular database to access other databases. Typically, middleware programs provide messaging services so that different applications can communicate. The systematic tying together of disparate applications, often through the use of middleware, is known as enterprise application integration (EAI) (Web ref. 20).
Raw data	• Raw data (also known as primary data) is a term for data collected from a source. Raw data has not been subjected to processing or any other manipulation, and are also referred to as primary data. Raw data is a relative term (see data). Raw data can be input to a computer program or used in manual procedures such as analyzing statistics from a survey. The term can refer to the binary data on electronic storage devices such as hard disk drives (also referred to as low-level data) (Web ref. 23).
Metadata	• Metadata is "data about data". Structural metadata is about the design and specification of data structures and is more properly called "data about the containers of data"; descriptive metadata, on the other hand, is about individual instances of application data, the data content (Web ref. 23). As information has become increasingly digital, metadata are also used to describe digital data using metadata standards specific to a particular discipline. By describing the contents and context of data files, the quality of the original data/files is greatly increased (Web ref. 23).
Context	• Background, environment, framework, setting, or situation surrounding an event or occurrence (Web ref. 5). • In computer science, a task context (process, thread ...) is the minimal set of data used by this task that must be saved to allow a task interruption at a given date, and a continuation of this task at the point it has been interrupted and at an arbitrary future date (Web ref. 23).
Analytical Context	• In this work the analytical context is a minimal set of data and metadata, needed to describe, define the analytical procedure (and if necessary reproduce it).