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Executive summary report

OSCAR

Optimal Systems-in-Systems Control and Architecture

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Model Based Cybernetics Software for the Control of Complex Systems

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Executive Summary report

Biological or bio-inspired systems are known to be complex to model, due to their nonlinearity, extremely high dynamic range, susceptibility to environment and potential self-adaptation. The overall objective of the Model Based Cybernetics Software for the Control of Complex Systems (OSCAR) project was to provide an overview of the modelling challenges related to bio-inspired systems and suggest potential additional characterization and model elaboration to achieve generic conclusions leading to an integrated vision of simulation and control of complex systems. This is the framework of OSCAR summarized by the highlight: modelling of bio-inspired systems.

More precisely, the scope of OSCAR is man-made Life Support Systems (LSS) with the sake of conceiving and operating a LSS, fulfilling operational constraints and minimizing the volume and mass that are necessary. The application to the Micro-Ecological Life Support System Alternative, MELiSSA, which has been the LSS project supported by ESA for more than 30 years, is the perfect challenging example of application of the methodology proposed in the framework of OSCAR.

MELiSSA is an international collaborative effort gathering 15 partners and led by the European Space Agency (ESA), with the objective of developing a circular life-support system to support long-term human space missions. It is a semi-closed loop striving for recycling and recovering oxygen, water, and food from waste with minimum on-board extra resources and minimum mass buffers.

The general structure of the MELiSSA loop is inherited from a natural ecosystem and the detailed structure depends on the application and on the context. The loop is composed of interacting bioreactors, separators, higher plant chambers and a crew compartment. It must be considered as an integrated sum of interconnected unit operations into a circular system, including biological compartments.

A key guideline of previous MELISSA activities driven by the MELiSSA consortium has been a generic approach and the development of a general methodology for tackling so-called circular systems. On one hand, all unit operations in charge of the elementary functions constitutive of the entire loop need to be studied, up to a thorough understanding, and translated into mathematical models. On the other hand, the systemic approach of complex, highly branched systems with feedback loops must be performed. This entails to study in the same perspective, with the same degree of accuracy and with the same language and concepts, waste degradation, water recycling, atmosphere revitalization, food production systems, etc., prior integration of knowledge-based control models, organized in several hierarchical levels with a decision system interface with human environment. Intelligence of the system is based on the adequacy of the models for representing each unit operation and their interrelations in a suitable degree of accuracy and adequate range of validity of the models for implementing a hierarchical strategy of control. The models must well represent the primary interactions and must be sensitive to some input variation or some factors, otherwise they will not be representative of the system and will be useless. Numerical simulations should be considered as a tool for analyzing the effects of various parameters on the model performances and extend the model reliability to different operational ranges.

The modelling requirements are established at two levels:

- **At system level**, the requirements are defined considering the LSS at a whole. This is considered in a specific evaluation grid: the **A**dvanced **Li**fe Support **S**ystem **E**valuator (ALiSSE) is the starting point of any generic evaluation of the LSS.
- **At compartments level and for each unit operation**, the modelling requirements are established at a generic level, whatever the layer.

Importantly, the guidelines for all requirements are the deterministic modelling[1], including mass and energy balances and the mechanistic approach[2] at different scales as an essential point generating the capacity to infer a control strategy based on knowledge models.

One key point for the structure that has been proposed and developed for OSCAR is to organize a way to make available throughout the model:

- The constraints imposed in terms of functions of a Life Support System.
- The mechanistic knowledge of the different elementary processes.
- The information about the structural assembly of the processes.
- The strategy of control of control for operating reliable and sustainable systems

OSCAR objectives

The objective of OSCAR is to provide an overview of the modelling challenges related to bioinspired systems, and identify additional characterization and model elaboration. The model-based approach, which is currently limited to an assembly of independent processes, is revisited and consolidated at system level.

OSCAR mainly follows a bottom-up approach. It is formulated as a complete revisit of the existing modelling and control issues of LSS with the objective to achieve generic conclusions leading to an integrated vision of simulation and control of complex systems. The objective is to move from a "model-based approach currently limited to an assembly of independent processes toward system level" and to "demonstrate the benefits of the transition from circular to a network system". The novelty and the most challenging points of the study are globally two-fold:

[1] As opposed to stochastic. Deterministic models enable to predict the outcomes. See complete definitions in TN 137.4.

[2] As opposed to empirical. Mechanistic models enable to understand underlying mechanisms and accumulate knowledge. See complete definitions in TN 137.4.

- Progressive integration of the complexity of the system from layer to layer in a bottom-up perspective;
- Reverse (descendant or top-down) flux of information, from the system level to the components and the elemental mechanisms, in order to generate a *model-based cybernetics* approach supporting the concepts of self-organisation, bio-inspired systems and also Artificial Intelligence (AI).

The general organisation of the structure of understanding and modelling is schemed in the arborescence described in Figure 1. This figure represents the complexity tree that has played the role of a common thread throughout the work of OSCAR deployment.

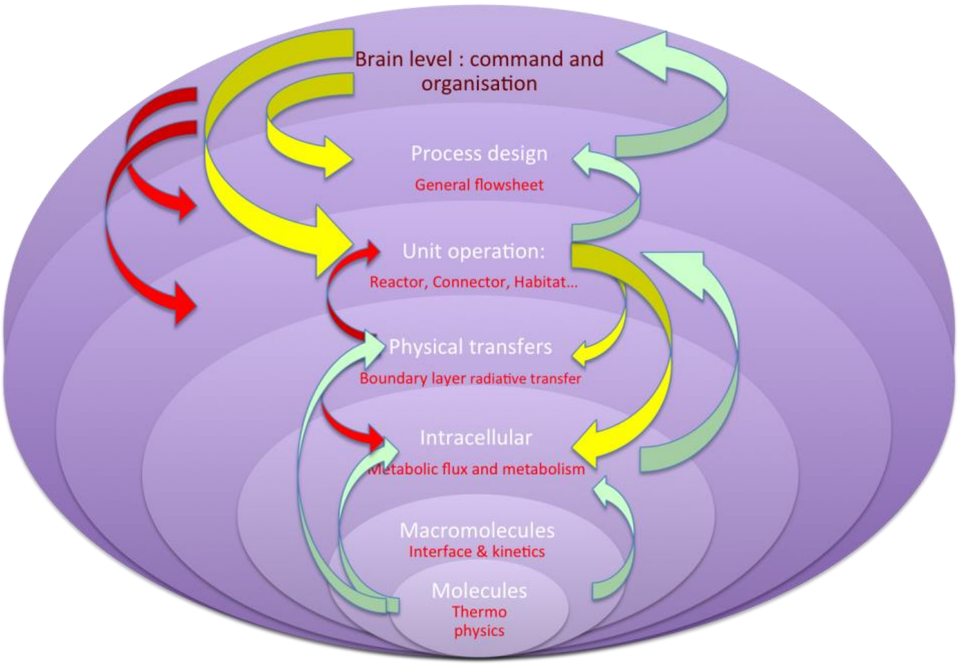

Figure 1 : Complexity tree: from molecule to LSS. The "System-in-System" organisation. Colour code: yellow means information request; green means simulation results & sensors outputs; red means constraints, control & architecture.

Briefly the seven layers interplay in the following sequence:

- L1 and L2 are related to compounds properties (thermophysical properties, kinetics and interfacial properties at molecule and macromolecule levels).
- L3 and L4 are related to local phenomena description (metabolism and physical transfers).
- L5 and L6 are related to integration (unit operation and process level).
- L7 is the brain-level and the decision maker system.

OSCAR works structuration

The OSCAR works have been divided into three main tasks:

- Task 1 deals with the elaboration of modelling requirements of bio-inspired systems (TN 137.1);
- Task 2 deals with the identification of modelling limitations and critical issues (TN 137.2);
- Task 3 is the application to a concrete case of coupling three compartments of the MELiSSA loop (CIII, CIVa and CV) and operating the previous concepts to a case study (TN 137.3.1 and TN 137.3.2).
- A final fourth task summarizes the main recommendations for future studies and deployments (TN137.4).

OSCAR outcomes: definition of modelling requirements (TN 137.1)

The general formulation of the modelling requirements has followed the general structure:

- Functional requirements
  - MUST
  - SHALL

- Operational requirements
  - MUST
  - SHALL

- Interface requirements
  - MUST
  - SHALL

- Constraints requirements
  - MUST
  - SHALL

The requirements have been detailed for each of the seven constitutive layers presented in Figure 1 and at system level, adopting a bottom-up presentation.

This makes a list of 4 x 2 x (7 + 1) = 64 tables describing the development structure of OSCAR and drawing a global network of transfer of information, decisions, results, constraints, structural laws, and structured modelling between the various parts of LSS system. The requirements list includes the interactions between the different levels of description.

This requirements list must be read as an oriented graph, a requirement at a certain level (or layer) being in resonance with another in another layer and finally at the system level. The main construction supported by Figure 1 results in system-in-system topology.

The bottom layers, from 1 to 3 are the layers that support basal information about elementary processes, whatever they are chemical, physicochemical, or biological. They can be understood as sources of data. These layers are essential and require the attention, knowing that wrong data will necessarily lead to wrong estimations and simulations. They cannot be considered only as database, the requirements being specific to the objective of Life Support Systems, involving living organisms, complex molecules, aqueous solutions, etc.

The intermediate layers, 4 and 5, are the layers where the main models and sketch of the reality are formulated. This concerns by example, physical transfers (mass, energy, radiation, and momentum) and through their integration throughout a unit operation.

The last two layers 6 and 7 are the layers where the process is assembled. L6 supports process assembly and conception. L7 supports decision making system and information storage.

Also, the requirements in terms of models' reduction (surrogate models) are an extensive part of the requirements definition. This is of special importance for developing a system architecture that remains tractable on a simulation poi t of view.

The previous list of requirements concerns essentially models developments and simulation of different configurations of LSS. Of course, this will have to be associated to other points that have been so far skipped and will remain to be added. This is the case of sensors developments and real-time diagnosis of a working process with an enrichment of the models with the experimental observation of real processes. This is also the case with structuration of the simulation results and of the decision-making procedure, which remains up to now as a "requirement." The interface with artificial intelligence procedures has not treated here. However, it is completely in-line with the above structure of OSCAR. It is known as an up-to-date essential question in process developments, indicating that OSCAR structure goes beyond the strict applications to LSS.

OSCAR outcomes: identification of modelling limitations and critical issues (TN 137.2)

OSCAR mainly follows a bottom-up approach. A selected academic study case (e.g., a MELiSSA loop restricted to: nitrification, photobioreactor and crew) has been considered to investigate and demonstrate the benefits of a transition from a circular to a network system.

After identification of modelling limitations and critical issues, the state of art of presently MELiSSA running models for the different compartments has been investigated. This includes:

- The kinetic assumptions regarding biological kinetics and physical kinetics (gas liquid transfers, light energy transfer models);
- The models' logics;
- The models' reduction;
- The control command of the different compartment at MPP.

The integration of the compartment models into a global model including the local control algorithms and the global control strategy of the loop has been studied. The choice of language and simulation environment is discussed, considering the choice of the MELiSSA community.

From the analysis of the developed works on CIII, CIVa and CV, that is already a complex system, it is recommended to let the experts of each domain choose their simulation tool and to set up an integration process in a co-simulation tool for the global system model. By example, when it is necessary to use CFD tools to understand the details of physical constraints in terms of transfers and mixing (layer L4) it is recommended to use specific software for CFD. For the process simulation, specific tools such as ProSim, ASPEN, g_PROMS or even Simulink can be used (layers L5 - L6). For the control system, tools such as Simulink, AMESim or Dymola for the system level can be used. It is outlined that the development of the composite model can be done in Simulink, using the S-Functions interface or with a co-simulation environment with the FMI standard.

For reasons of flexibility and modularity, the MELiSSA consortium has chosen Simulink for the modelling of the compartments as well as for the modelling of the global loop connecting the compartments to the hardware network and the control system. It is emphasized that this choice is compatible with the methodology for defining the architecture of the control strategy, which specifies the organization of the model as well as the interfaces between compartments on the one hand and between compartments and control on the other hand. This proposed organization allows to use, according to the need, static models of the compartments or more complex but more realistic dynamic models.

However, this organization must still be adapted to incorporate and adapt the structure of modeling and simulation of chemical and biochemical engineering processes, namely the knowledge coming from the bottom layers L1 and L2 and also L3 when referring biochemical and microbial processes. These specific requirements for biological conversions must be tackled and understood at the process simulation level.

OSCAR outcomes: Toward the performance analysis of MELiSSA bioreactors with Computational Fluid Dynamics (TN 137.3.1)

The CIVa compartment is one of the best known in the MELiSSA loop. The theoretical and experimental studies that have been realized on PBR operation in the framework of MELiSSA experiments have shown that this compartment could be controlled by acting on the light energy supply and on the liquid flow rate (dilution rate). Nevertheless, in order to get a broader range of operational conditions and a more thorough understanding of the influence of the variation of some process variables on the performance of the PBR, work still needs to be done for tuning its mathematical description. One important limitation of the on-going models is that the microalgae are supposed to face homogenous liquid concentrations, though the heterogeneity of the light energy distribution has been demonstrated to play a key role and is currently taken into consideration in all culture simulations. To address eventual liquid (and dissolved gas) heterogeneity, CFD simulations are needed. The aim of this study was a first step towards broadening the range of knowledge of PBR performances.

The MELiSSA Pilot Plant (MPP) in Barcelona photobioreactor (PBR) is considered and briefly described to introduce its role in the MELiSSA loop and its functioning and design. Some experimental data available from previous TNs in the context of MELiSSA Pilot Plant projects are also reviewed. The advantages of using CFD to analyze the performances of bioreactors are summarized, together with the description of the peculiarities of CFD applied to multiphase flows, which are often encountered in bioreactors. The simulations carried out with the CFD software Ansys Fluent and the analysis of the results are described.

In particular, experimental results in terms of hydrodynamic and mass transfer characterization are obtained and discussed. The CFD simulations of the CIVa compartment carried out with the software Ansys Fluent are presented with the objective of highlighting the potential benefit of using CFD to obtain essential information for characterizing the gas and liquid flows into the reactor volume and the mass transfer properties of the reactor.

The output of this work will guide future project efforts, take could aim to:

- Take into account the bubble size distribution in the simulation through the Population Balance Model
- Validate numerical simulations with specific experimental tests.
- Extend the CFD characterization of the CIVa compartment to other operational conditions.
- Exploit CFD simulations to characterize other reactors inside the MELiSSA loop.

Three important points are highlighted:

- The above CFD simulations of gas liquid mixtures (air and liquid broth) use a supposed diameter of bubbles. It must be extended to a bubble size distribution.
- The CFD simulations have the interest to provide the values of the gas liquid transfer coefficient (K_La) and of the liquid recirculation velocities, opening the door to define a detailed description of the liquid environment of the cells.
- In any case, the CFD simulations *per se* cannot be used in a complex and complete process simulation, calling for a systematic work on the way to derive surrogate models from such detailed descriptions. This last point is clearly an important point to treat for a complete development of OSCAR methodology.

OSCAR outcomes: methodology for system simulations through reduced order models: an application to the C3-C4a-C5 MELiSSA loop (TN 137.3.2)

Following the conclusions of previous TN 137.3.1, the introduction of a reduced order model technique, i.e. the construction of surrogate models, in the context of the system simulation of a portion of the MELiSSA loop is examined.

Targeting the system simulation of a reduced part of the MELiSSA loop (CIII – CIVa – CV), the benefit of introducing a reduced order model of the CIVa photobioreactor (PBR) into the system simulation is analyzed. The CFD simulations are the starting point for the implementation of a reduced order model of the PBR. The motivation, theory and benefits of using reduced order models are also discussed.

The proposed approach for the development of reduced order models of the MELiSSA CIVa compartment uses the Ansys Workbench DesignXplorer Toolbox. At first, the workflow for the model generation is introduced. Then two different types of reduced order models are generated: a 3D reduced order model and a Response Surface reduced order model.

It is demonstrated how complex 3D CFD simulations describing the flow behavior of the CIVa photobioreactor can be translated into reduced models ready to be used in a system simulation tool, at an affordable computational cost. This methodology applied for reference to the MELiSSA framework, normally could be extended to other domains, as long as the interest is on sensitivity analyses of the effects of a change of design or process parameters on the system outcomes, to take full advantage of these recent progresses in data treatment and simulations.

In the same perspective, the system simulation of a partial MELiSSA loop, comprising compartments CIII, CIVa and CV is envisaged. After a brief description of the mechanistic models of these three compartments, the response surface of reduced order models is exploited to perform some system simulations.

As a guideline for future exploitations, the output of this work shows that efforts to be done take could aim to:

- Increase the number of design points to improve the accuracy of the CIVa reduced order model by performing more 3D CFD simulations
- Validate reduced order model simulations with specific experimental tests or 3D CFD dedicated simulations.
- Exploit reduced order models to validate system simulations in different sets of operating conditions
- Develop reduced order models of other MELiSSA compartment

OSCAR outcomes: recommendations for future works (TN 137.4)

Modelling and control of bio-inspired ECLSS is a process that combines complication and complexity.

OSCAR draws a global network of transfer of information, decisions, results, constraints, structural laws, and structured modelling between the various parts of LSS system. It has been conceived as a tool for doing progressively implementations and refining understanding and knowledge on the system translated into mathematical models. This was the primarily objective of OSCAR.

From the complete list of requirements for installing the methodology, the identification of modelling limitations and critical issues has been done. Application of advanced models has been studied for the special case of using CFD simulations in the case of the MELiSSA pilot plant PBR. Then, the way to install reduced order models (or surrogate models) has been investigated.

From this work, a complete list of recommendations has been established and classified, both for each layer and at system level. Importantly, there is a strong recommendation for pursuing training of the MELiSSA community to the OSCAR methodology. There is also a strong recommendation for tuning a software platform for developing modelling and simulation tools, knowing that a generic tool is not yet in use in the Life Support System community and needs to be chosen and used. Among other, there is a specific need for transient and dynamic simulation software, that is still lacking.

The interface with artificial intelligence procedures has not treated in OSCAR project. However, it is completely in-line with the above structure of OSCAR. It is known as an up-to-date essential question in process developments, indicating that OSCAR structure goes beyond the strict applications to LSS.

Two final remarks must be highlighted.

- The model definition: a model is a formal object that is an expression of the reality as sketched by the modelizer. The translation of a model is generally a set of equations or a set of logic rules. The numerical resolution of the previous set of equations or logic rules leads to the results of the simulation. The final expression is a software package. In any case, the four previous things – formal object; set of equations; numeric resolution; software package – must not be confused.
- Several times in the previous requirements list, the term 'degrees of freedom' has been invoked. This is a crucial point as it is generally associated to the dimension of a problem (or the dimension of the regulation space). Nothing has really been yet presented in this TN about the determination of the degrees of freedom and of their number. The experience shows that it closely related to the models' hypotheses, the degrees of approximations, the mode of expression. It has to be considered that it is a key point for considering the solvability of problem. This has to be envisaged first at unit operations levels considering several degrees of hypotheses, structuration of models, etc. prior developing the same reasoning structure at the overall system level.