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Executive Summary

Within HYDROPTICS project optimization steps to be discussed include two main aspects: optimization of the automated liquid-liquid extraction process and optimization of the key process steps in the water purification plant.

Work on this project task will mainly deal with the elaboration of the system requirements and its conceptual design. One of the key points is to collect required input to come up with a digital twin of the complete industrial process where Computational Fluid Dynamics (CFD) simulation methods will be implemented.

Within this deliverable the Know-how in chemical engineering will be applied. Whole work will be supported by CFD simulation and process simulation for modelling of complex chemical processes (multiphase).

Table of Contents

1. Introduction

In the field of gas and oil production, the requirements for an exact and fast measurement of the water quantities arising in the process and their properties are of utmost importance for the overall efficiency of the processes. In order to achieve this increase in efficiency, the most precise and timely monitoring of process variables are required, which is a driving force behind the research in the HYDROPTICS project.

To achieve such an accuracy in monitoring, a precise knowledge of the individual process steps in the field of measurement technology as well as in the overall process is necessary. For this reason, different thermodynamic and hydrodynamic simulation methods are to be applied in order to contribute to the development of various measuring methods and the optimization of the plants. The analysis by means of simulation can be divided into the two areas of computational fluid dynamics and process simulation. Project requirements will be investigated in order to select adequate simulation processes.

Within HYDROPTICS process of optimization two main aspects will be researched:

- Optimization of the automated liquid-liquid extraction process
- Optimization of key process steps in gas- and oil separation units and water purification:

2. Optimization of liquid-liquid extraction process

In process, and every other industry major concern is to improve the quality of products and services. The research to be conducted within HYDROPTICS involving advanced Computational Fluid Dynamics (CFD) simulations concerns on-line sample preparation techniques. Main target is to assure proper integration into the industrial process.

With regard to this task the process of liquid-liquid extraction will be investigated. This complex process, having two involved unit operations – extraction and phase separation will be investigated and optimised for its purpose.

Fig. 1 represents the workflow regarding the optimization of liquid-liquid extraction process. Project requests will be investigated in detail followed by completed literature research. Next step will be design of 3D model with determination of all necessary parts. Crucial steps that come after designing model are prototyping and CFD simulation. These two steps will be done almost parallel with aim to receive prototype which can be tested and validated with CFD model. Such approach of building prototype that will be simulated will allow testing, validation and highly important process of optimization.

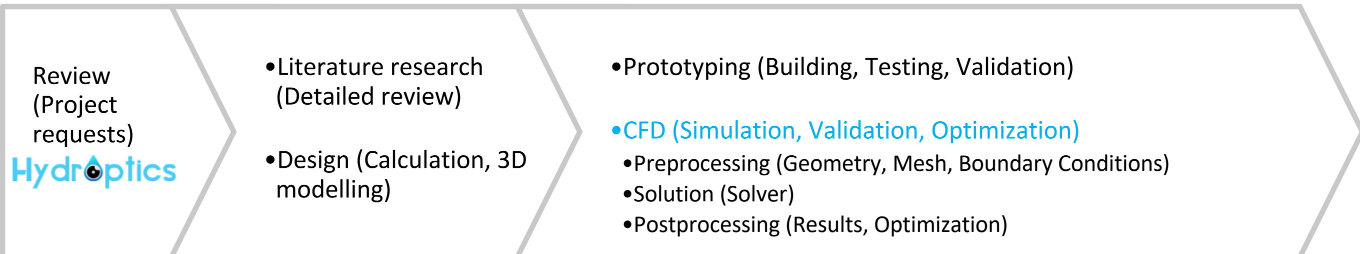

Fig. 1: Workflow of optimization of liquid-liquid extraction process.

The optimization process will be supported by CFD methods in order to derive a digital twin model. Using CFD approach will allow variation of throughput and solvent/water ratios and further support to optimization process.

2.1. Computational Fluid Dynamics in Multiphase flows

Multiphase flow refer to any fluid flow that consists of more than one phase or component. In industrial applications multiphase flows are very common. Thus, it is highly important to make investigation in detail so it becomes possible to predict the behavior of such systems. Additionally it leads toward possibility of optimization of such systems for their best performance.

Verified simulation tools and methods can provide a detailed insight at reasonable time and cost frame. CFD can give a full spatial and temporal representation of multiphase systems.

Use of CFD, different multiphase phenomena can be investigated and interpreted to help improving the process. In order to make suitable multiphase simulation the discretization (mesh) should be fine enough to capture all the flow and the phase structures. This is usually computationally very expensive.

For CFD simulations, it will be used OpenFOAM®, free, open source CFD software. Extensive range of features is developed and implemented for solving of different complex fluid flows. The models are to be validated against experimental fluid dynamic approaches and used in simulating wide range of applications. CFD knowledge will be deepened and the suitable multiphase solver for modelling will be selected.

2.2. Requirements on process optimization

In CFD modelling of complex multiphase chemical processes, requirements needed for simulation will be elaborated. One of the key aspects to be discussed are requirements for selection of optimal sampling points. Such discussion will be made in close cooperation with industrial end-users.

2.2.1. On-line sample preparation

Within this task of HYDROPTICS project process of liquid-liquid extraction will be investigated. The two involved unit operations are:

- extraction
- phase separation.

Work on both units will include process of optimization in order to fulfill efficiency, speed and ruggedness requirements. The optimization will be conducted based on CFD simulation and chemical engineering process. In this regard, new strategies for continuous extraction and phase separation process and application in the ml/min scale will be investigated.

2.3. Extraction and phase separation

Liquid-liquid extraction and phase separation will be investigated with aim to minimize the amount of solvent (cyclohexane) used for this purpose. Such complex process needs to be reliable. Key targets are:

- robust and stable operation
- high organic phase recovery (to minimize solvent loss to water).

On a large scale, 3-phase decanter and 3-phase separators do exist and can be applied in process of separation. The aim within this project is to miniaturize the concept for different feeds as needed for sample preparation. As those separators are not present in miniaturized concept the research on this topic is needed to be conducted in detail. The design step will be strongly supported by CFD to receive a digital twin which allows the variation of throughput and cyclohexane/water ratios.

3. Process Simulation and Optimization of key processes in gas- and oil separation and water treatment for secondary water re-injection

The overall process of gas and oil separation in secondary oil recovery facilities has a number of unpredictable characteristics that affect the overall effectiveness of the plant components. Not to be neglected is the quality of the water produced, which has an influence on the overall effectiveness of the plants during further injection. The basis of the HYDROPTICS project is to enable good monitoring of the properties of this water. For this purpose, an exact understanding of the processes the water goes through is essential. These processes comprise a multitude of individual components which have a large influence on the dynamics and quality of the water produced.

For this reason, the test facility is analyzed with the help of process simulation methods as well as individual CFD processes in order to gain a more precise understanding of these facilities. By means of the simulation data, the simulated data will subsequently contribute to the increase of the measurement effectiveness as well as to process optimization.

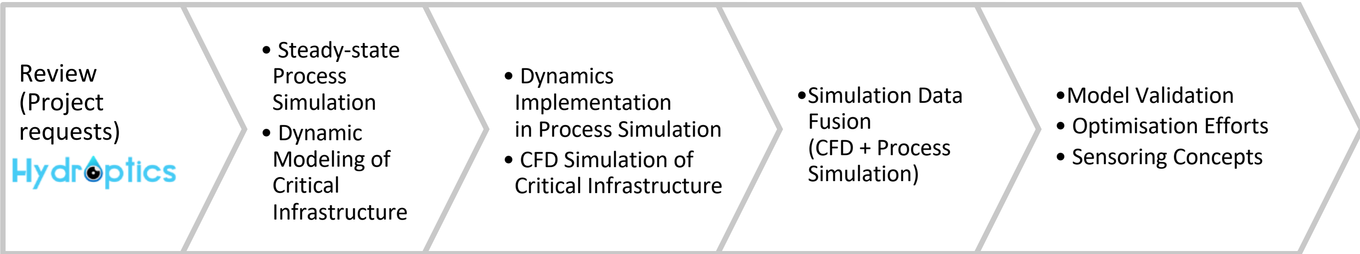

Fig. 2: Workflow of Process Simulation and Optimization.

The workflow chart above shows a sequence of methods which are used for the simulation of the plants and are explained in the following sections.

Therefore the process simulation task is divided in 2 areas:

- **Dynamic Process Simulation**
  - In close collaboration with OMV, the generated model will represent the real-life test facilities and will contribute to boost the research in sensing concepts within HYDROPTICS project and the application of optimization strategies.
- **CFD Simulation of Relevant Components**
  - Parameters of critical process components will be evaluated more closely with the help of CFD simulations.

3.1. Process Simulation

The scope of the process simulation aspect will cover the entire plant while relevant components will then be simulated by implementation of custom modeling. This approach will result in a deeper knowledge of the plants operating parameters and will also allow to enhance the sensing concepts applied within the project. Furthermore the application of optimization strategies will be carried out on the simulation model, in order to be able to contribute to increasing the efficiency of the overall system.

The scale of the simulation will include the overall process, so a vast majority of the different parameters within the water processing and treatment cycle will be evaluated. The first step of this approach will be to build a digital twin of the test facilities. Since the process of gas- and oil separation inhibits a large amount of dynamic behavior within distinct plant components, the focus of this step will be the simulation of the dynamic effects of the parameters within this distinct components. The exact workflow of generating such a digital twin can be seen in Fig. 2.

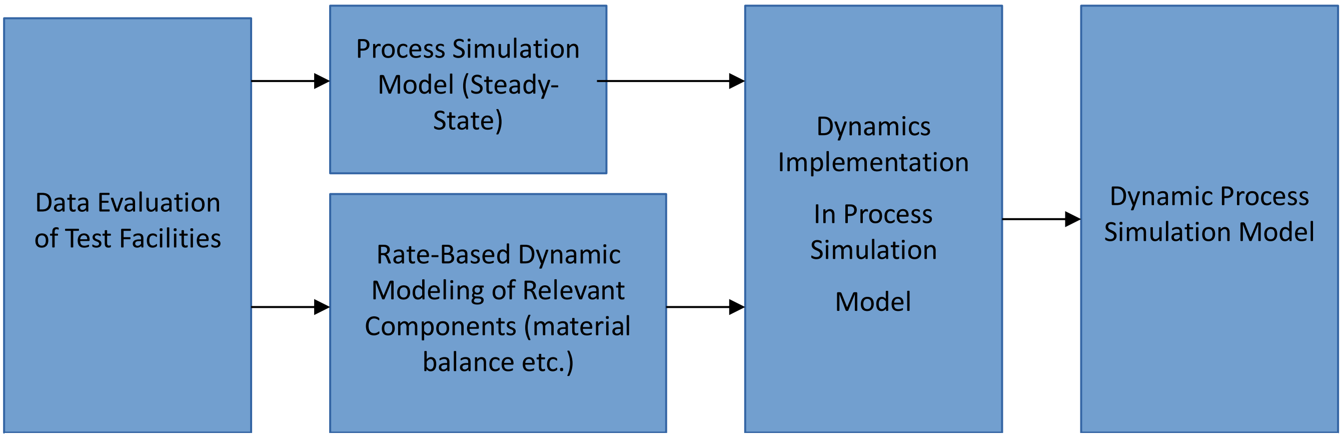

Fig. 3: Workflow of the first task in process simulation: "Establishing a Digital Twin"

The selection of the relevant plant components is coordinated with the operating company of the test facilities. Also the selection of the dynamic modeling concepts will be chosen on to focus on the most relevant parameters to provide the greatest possible support to the photonics measurement units.

The model itself will also serve as a basis for the application of later optimization strategies and data evaluation methods. The fluctuation of water inflow rate and the overall inflow composition will be simulated and the gained data will then be used to optimize the response of the involved components to the altering dynamic properties.

3.2. CFD Simulation of Critical Components

In order to enhance the performance of the simulation process, CFD simulations on relevant plant components (components which include a vast majority of transient behavior) will be carried out. This task will include the identification and modeling of these components. The components will be modeled exactly according to the test facility with the help data provided by the operating company. The CFD simulation will be carried using OpenFOAM® to provide a better insight of the transient fluid behavior in the selected process steps. The data gained from this simulations will be considered in the overall process simulation to boost the simulation efficiency.

Therefore, with the implementation of CFD simulation, process simulation will work as a basis for process optimization by considering CFD results of critical components through "direct subfunction calls of the CFD solver from process simulation providing boundary conditions" or "look-up tables from previously performed CFD simulation". These multi-scale approaches may be either applied to steady state modelling or transient (=dynamic) process simulation models.

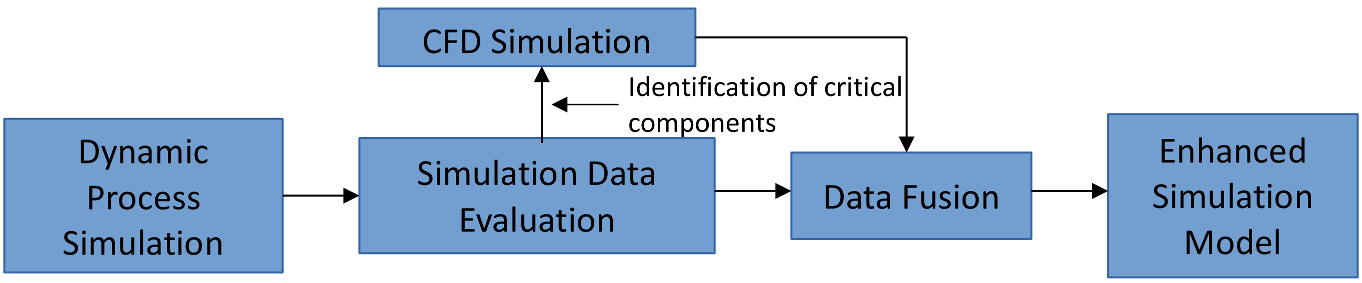

Fig. 4: Combination of Process Simulation and Computational Fluid Dynamics

The data gained from the CFD simulation gives an insight in different hydrodynamic phenomena which can not be represented by the process simulation model. This data will then be taken into account in the overall simulation.

3.2.1. Process Simulation Requirements

The purpose of the process simulation approach is to give a deeper insight of the parameters for different properties (e.g. hydrocarbon concentration in water) at all processing stages of the facilities. For the purpose of delivering the greatest possible accuracy of this simulation a close interaction with the project partners and operating company will be carried out.

3.3. Optimization strategies based on process simulation

The digital twinning concept allows to determine the plants behavior for different operating parameters of the plant. Since the dynamic behavior often leads to undesired effects in the larger scale of the plant, these unwanted operating points will be evaluated with the established digital twin. De-Bottlenecking strategies, in order of altering the controller response in the affected components, are able to increase the performance of the facilities. Also methods to determine the water output quality will be integrated in the simulation process. This concept of process simulation and digital twinning will be carried out from the beginning with the idea of using this digital twin for further process optimization.

3.3.1. Optimization Strategies Requirements

The optimization measures (benchmarks) are determined in close cooperation with the project partners. Furthermore, the requirements of plant operators in the field regarding these measures will be considered.

3.3.2. Implementation of data from online measurements into process simulation

The data gathered by the photonic measurement systems applied in the overall process are able to give an insight of different states within the process, whereas the established mathematical defined process simulation model characterizes the overall structure of the plant. The raw data gathered by the sensors are often incomplete and redundant. Also the data can show a various number of errors and deviations. In order to enhance the quality of the measured data and to improve the sensors and overall measurement concept, a deeper analysis of the data is necessary. In this concept, both existing online measurements (e.g. flow sensors, temperature and pressure sensors) in combination with new Hydroptics sensor development will be combined to calculate the material balances for use as process simulation model calibration and validation data.

In a second step, using the DVR (Data validation and reconciliation) method, the data of the online measurement will be analyzed and a data set, which is representing the system state more precisely, can be specified. The established Digital Twin of the process can be consulted for the validation of the data and to further enhance the reconciliation algorithms. Implementation of reconciled data sets in the used process simulation software are also carried out to achieve more accurate digital twinning of the facilities.

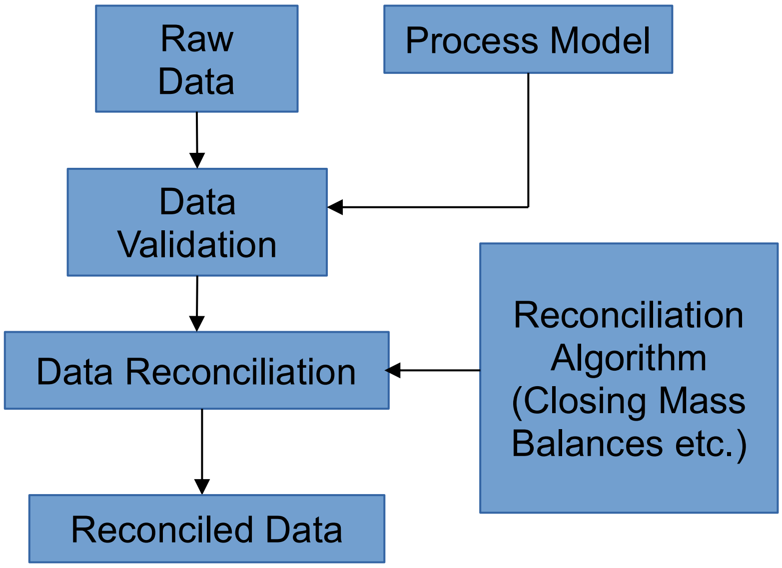

Fig. 5: Data Validation and Reconciliation Workflow

With DVR applied on real world process data, a more precise calibration of sensor and measurement equipment and therefore more consistent measurement data can be achieved. Also the reconciled data will be used to enhance the overall performance of the dynamic simulation model, in order to achieve a model which best corresponds to the real plants. The used reconciliation and validation methods depend on the different locations of the measurement systems. The locations of the sensors are coordinated with Hydroptics partners OMV and Tupras to achieve the best process control and measuring schematics.

Conclusions

The main areas in aspect of chemical engineering were defined to determine the starting point of the simulation approach based on the different tasks of the project applications.

In CFD modelling of complex multiphase separation processes, requirements needed for simulation will be elaborated. As one key task of HYDROPTICS is the optimization process, it will rely on CFD methods in order to get a digital model. This will allow variation of throughput and further steps in optimization process.

Regards the project simulation and optimization standpoint, it was decided to achieve the digital twinning of the test facilities by means of a double access approach both consisting general process simulation and CFD simulations. Optimization strategies will then be applied on this digital twin according the requirements of project partners.