Chapter I: Reminder of the acquired knowledge

I-1- Overview

Computer-Aided Design (CAD) refers to the collection and use of computer tools (hardware and software) that enable the geometric modelling of an object, in order to conduct various tests on the product before its actual production or modification, or any related objective. To achieve this goal, various software and modelling tools can be utilized.

Furthermore, with computer-aided design, it is possible to create a 2D or 3D model of an object to visualize its appearance, functionality, and behaviour. Potential modifications to the object can also be made before its actual realization. The term "design" involves a set of iterative steps that facilitate the design and modification of an object to meet predefined objectives and comply with a set of constraints.

Therefore, by utilizing CAD, various tasks can be performed in the object design process, such as:

- Creating the primary model of the object
- Conducting different analyses and tests
- Constructing prototypes
- Making modifications and improvements
- Realizing the objects

Additionally, to acquire a CAD tool, only a few materials are necessary, represented within a computer, regardless of its type and components, along with software capable of performing design tasks. Figure 1 illustrates the basic components required to obtain a CAD tool.

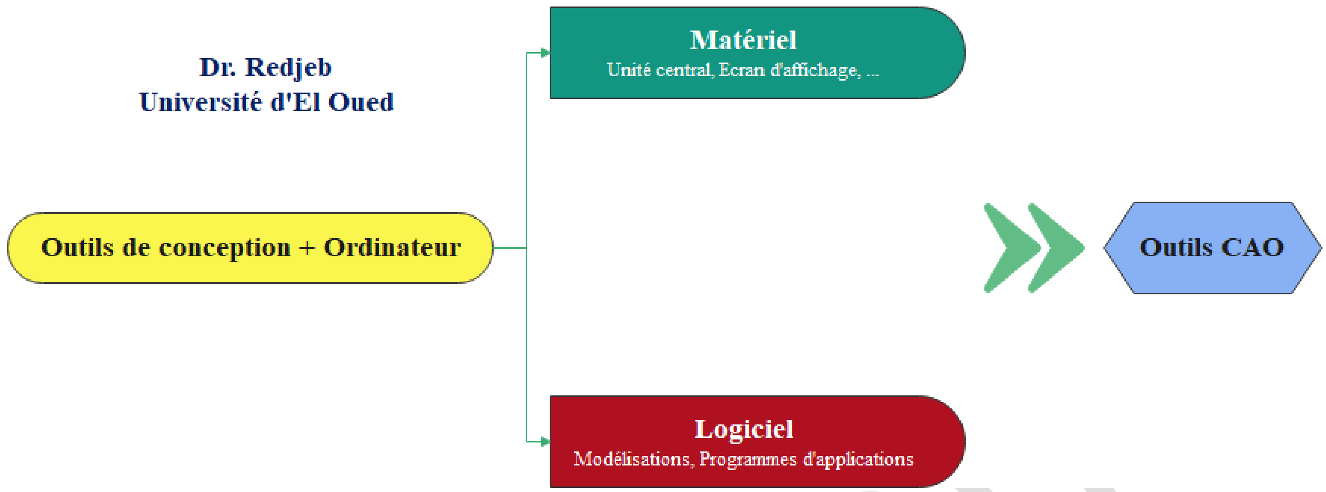

Figure 1. Hardware and Software Components of CAD

In process engineering, CAD encompasses numerous simulators ranging from specialized to robust and efficient process simulators, including Aspen Plus, Hysys, Chemcad, Prosim, etc. Through CAD, virtual simulations can be conducted before implementing a process.

I-2- Importance of CAD and Simulation

Over the past decades, computers have replaced traditional industrial drawing and design through the use of invented methods known as computer-aided design (CAD). Through CAD and simulation, every application in process engineering begins with a general description of the physical problem, which is then mathematically contextualized for computer representation.

In today's world, computer-aided design technology has proliferated and is utilized in almost the majority of fields where design and engineering are essential, such as architecture, civil engineering, chemical engineering, process engineering, petroleum engineering, and more.

However, it may take on alternative names depending on the specific field of application, such as:

- Architectural Computer-Aided Design (ACAD)
- Computer-Aided Manufacturing (CAM)

- Computer-Aided Production Management (CAPM)
- Computer-Aided Product Design (CAPD)
- Computer-Aided Process Design (CAPD)
- Computer-Aided Process Engineering (CAPE)

I-3- Activities of Design and Simulation

According to the literature, three main distinct activities can be distinguished to aid the designer in realizing their design and simulation. These activities are listed as follows:

- **Analytical Tools:** Where the designer must use empirical formulas and equations derived from mathematical models during the creation of a model or during its analysis or modifications.
- **Information:** It is necessary to identify the various properties and characteristics of the model. This type of information is essential for completing the design accurately.
- **Communication:** Here, the designer must communicate or dedicate the results of their work to move on to the subsequent phases. For example, they must communicate the results of their primary model and calculations to make certain modifications based on previous designs or predefined results.

I-4- Necessity of CAD and Simulation

In fact, CAD is highly significant today and can be used, as mentioned earlier, in various domains due to its feasibility. The following points explain some reasons why CAD should be utilized in almost all domains:

- **Increasing Productivity:** CAD helps the designer visualize the product before its actual production through simulation. They can make necessary modifications and optimize production time as well as associated costs.

- **Enhancing Design Quality:** As mentioned earlier, through simulation, it is possible to create primary models and make modifications to ensure limiting design errors. By conducting necessary analyses using the required software, the quality and accuracy of the design can be improved.
- **Improving Communication:** The use of CAD systems provides better technical drawings, greater standardization of drawings, improved design documentation, fewer drawing errors, and high legibility of drawings.
- **Creating a Database:** By collecting previous results and using shared experiences, it is possible to create a database containing abundant information that helps in model improvement, starting from an advanced point rather than from scratch.

I-5- Advantages of Using CAD and Simulation

It is evident that the use of CAD offers numerous advantages. For instance, CAD enables the design and analysis of systems with a high degree of complexity, surpassing human capabilities, especially at the micro and nano-scales. Additionally, CAD allows for testing and monitoring the behaviour of the object before its production, along with many other advantages like short execution time and the ability to perform analyses, etc.

Figure 2 presents some common advantages of using CAD.

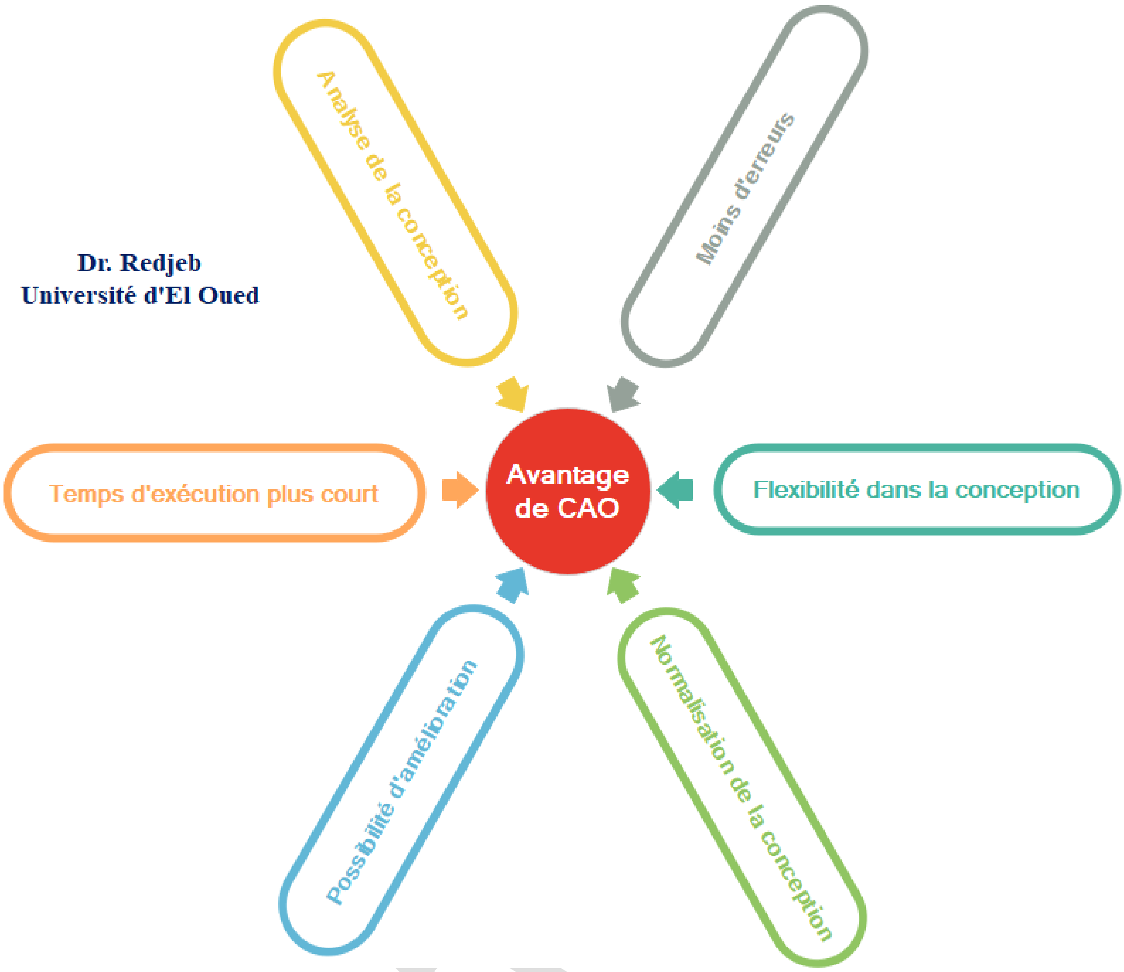

Figure 2. Advantages of Using CAD

I-6- Simulation and CAD in Chemical Engineering

Considering that the field of chemical engineering is characterized by process treatment, it is necessary to employ CAD by using specific simulation software to streamline processes, conduct pre-tests, make improvements to existing plants, and analyze and modify processes before applying them to installations. Therefore, simulation is of great importance in this field, and professionals or graduates in this field must possess at least basic knowledge of CAD.

However, in the field of process engineering, as a means of utilizing CAD technology, it is necessary to clearly define the objectives to achieve and conduct preliminary studies such as acquiring knowledge about constituents (physico-chemical properties, phase equilibrium, reaction kinetics, etc.). Subsequently, the process of designing a process or device comprises three main stages: synthesis, analysis, and optimization. The design process should proceed based on the desired and predefined objectives.

Figure 3 illustrates a typical flowchart for the various stages of CAD using a simulator.

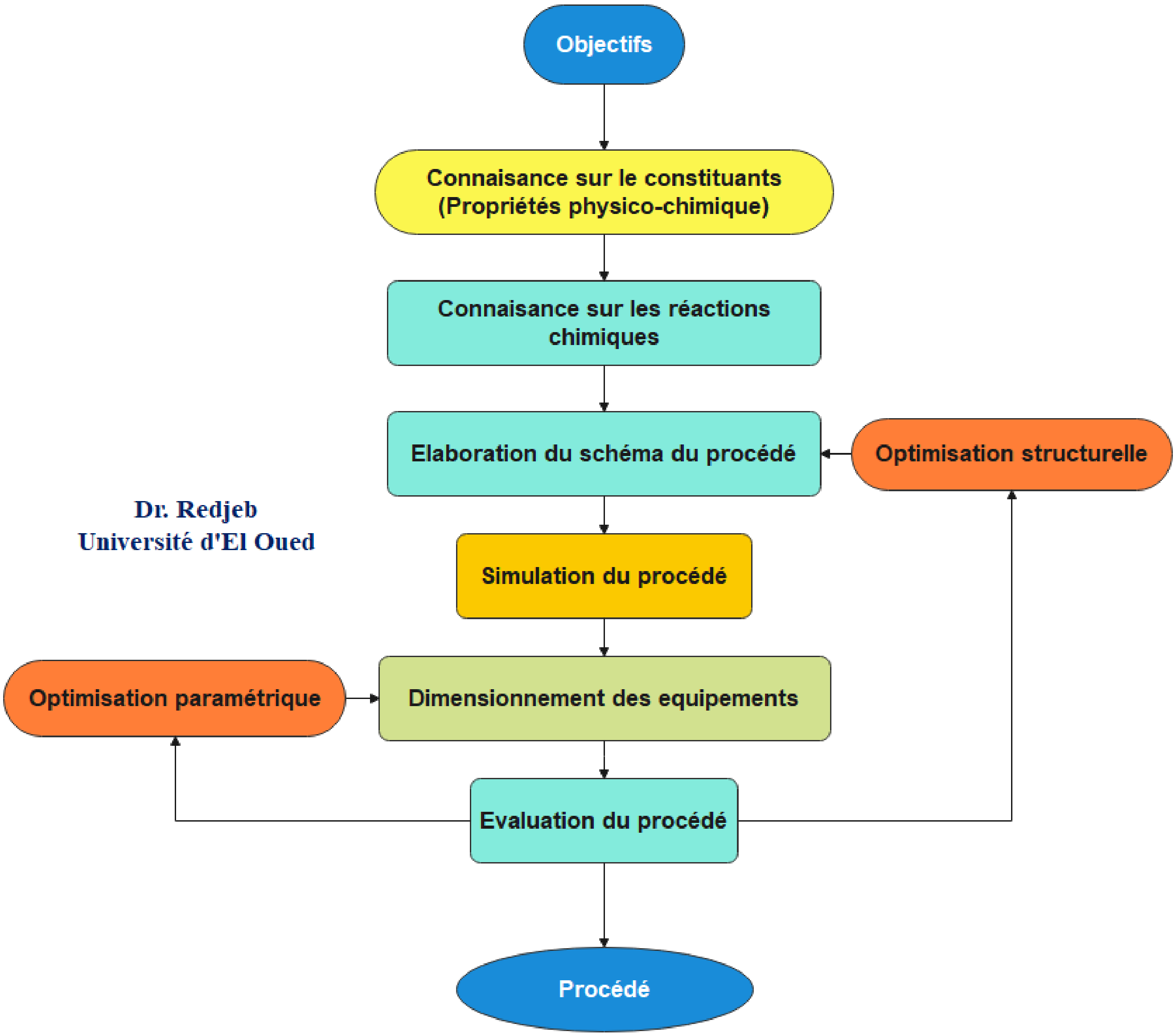

Figure 3. Different Stages of CAD

I-7- Simulation Software

Indeed, there is a wide variety of software used in CAD approaches. Among them, many are characterized by specific purposes such as process simulation or device design. In the context of chemical engineering and process engineering, there exists a diverse range of software, each with its specific features and applicability, including commercial and open-source software. Some of the notable ones include Aspen Hysys, Aspen Plus, Chemcad, Design II, Ideas, Indiss, Prosim (commercial), DWSIM, COCO, ASCEND (open-source).

Figure 4 showcases commercial software, while Figure 5 presents open-source software.

Figure 4. Commercial Software

Figure 5. Open-Source Software

1-7-1- Operation Modes of Simulators

Regarding the operation mode, two different modes can be distinguished:

- **Static Simulation (Steady State):**

As the name suggests, this mode means simulating a system in a static equilibrium, where its state variables no longer change. Static simulation of a process aims to define flow properties (flow rate, temperature, vapor fraction, etc.), as well as material and energy balances in a steady state, using different blocks representing various unit operations implemented in the simulator.

- **Dynamic Simulation:**

Dynamic simulation (or dynamic system simulation) involves using computer programs to model the time-varying behavior of a dynamic system. Systems are generally described by ordinary differential equations or partial differential equations. This mode of simulation aims to define stream properties over time during transient situations where the regime is not stable. In other words, it allows evaluating variables over time by solving systems of differential equations.

1-7-2- Conceptual Approaches to Simulation

According to conceptual simulation approaches, two different approaches can be distinguished: the first refers to the "**module-oriented**" (MO) approach, and the second is the "**equation-oriented**" (EO) approach.

The first approach, "**module-oriented**" approach, is the most widely used and adopted approach by the majority of commercial simulators like Aspen Plus, Aspen HYSYS, Chemcad, Pro/II, ProSimPlus, and DW Sim. In this approach, the basic element for building the process model is the unit operation model called a "module." It is the arrangement of unit operations dedicated to a specific function such as reaction or separation.

On the other hand, for the second approach, "equation-oriented" approach, EO simulators like Aspen Dynamics, gPROMS, and others are specifically dedicated to the dynamic simulation of processes. These simulators primarily act as solvers for systems of algebraic and differential equations.

In our case, the software adopted for this course is Aspen Hysys due to its high performance, features, and its applicability in various specific applications, particularly in this field, such as designing and simulating devices like columns, heat exchangers, pumps, and others, as well as constructing various processes.

I-8- Introduction to Aspen Hysys Software

Aspen HYSYS is the industry-leading process simulation software used by major oil and gas producers, refineries, and engineering companies for process optimization in design and operations.

Figure 6 displays the interface of Aspen HYSYS.

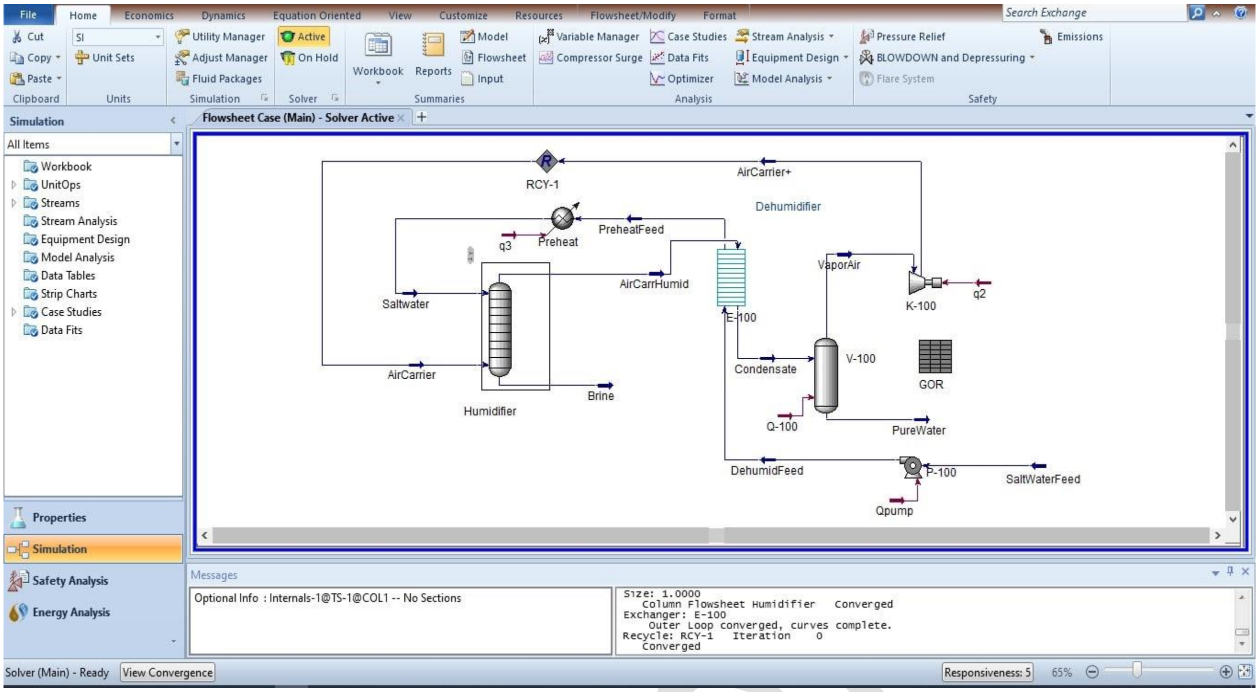

Figure 6. Aspen HYSYS Software Interface

This software is characterized by:

- A simple graphical interface for constructing process diagrams.
- Ability to perform various calculations with minimal required data.
- Automatic adjustment of calculation results with any changes in input data.
- Facilitation of error detection and corrections.

I-8-1- Performing a Simulation in Aspen Hysys

To perform a simulation in Aspen HYSYS, many steps must be followed, listed as follows:

1- Selection of Components: The Aspen HYSYS library contains numerous components classified into groups (traditional, hypothetical, electrolytes). They can be selected using filters and added to the component list in the simulated process.
2- Selection of Thermodynamic Model: One of the most important things is the selection of the fluid package, where the user must select the thermodynamic model to use for calculating chemical properties (density, enthalpy, etc.) and

phase equilibrium in streams and separation units.

3- Building the Process Flow Diagram (PFD): This can be done by selecting the desired units from the object palette and placing them directly on the process sheet. Additionally, all material and energy flows must be placed on the PFD. Each input or output stream is connected to a unit.

For a better understanding of the use of Aspen Hysys and to learn more about PFD, lab sessions are used.

1-8-2- Design of Various Devices (Columns, Heat Exchangers, Reactors, etc.)

As mentioned in the previous sections, computer-aided design allows for the design of various devices used in different processes, whether applied in the petrochemical sector, chemical sector, or any other domain. The selected software (Aspen HYSYS) enables the user to design different devices, such as columns, heat exchangers, and reactors, due to the extensive range of available data and components. The user can select the appropriate column from a set of different columns based on the case study, such as a distillation column, separation column, etc. Likewise, they have the choice to select the most suitable heat exchanger from different types, such as shell and tube, plate fin, etc., and the same goes for reactors (see Figure 7).

In line with this, relevant sessions dedicated to practical training will be assigned to understand the methodology of design and utilization of these different components using this software.

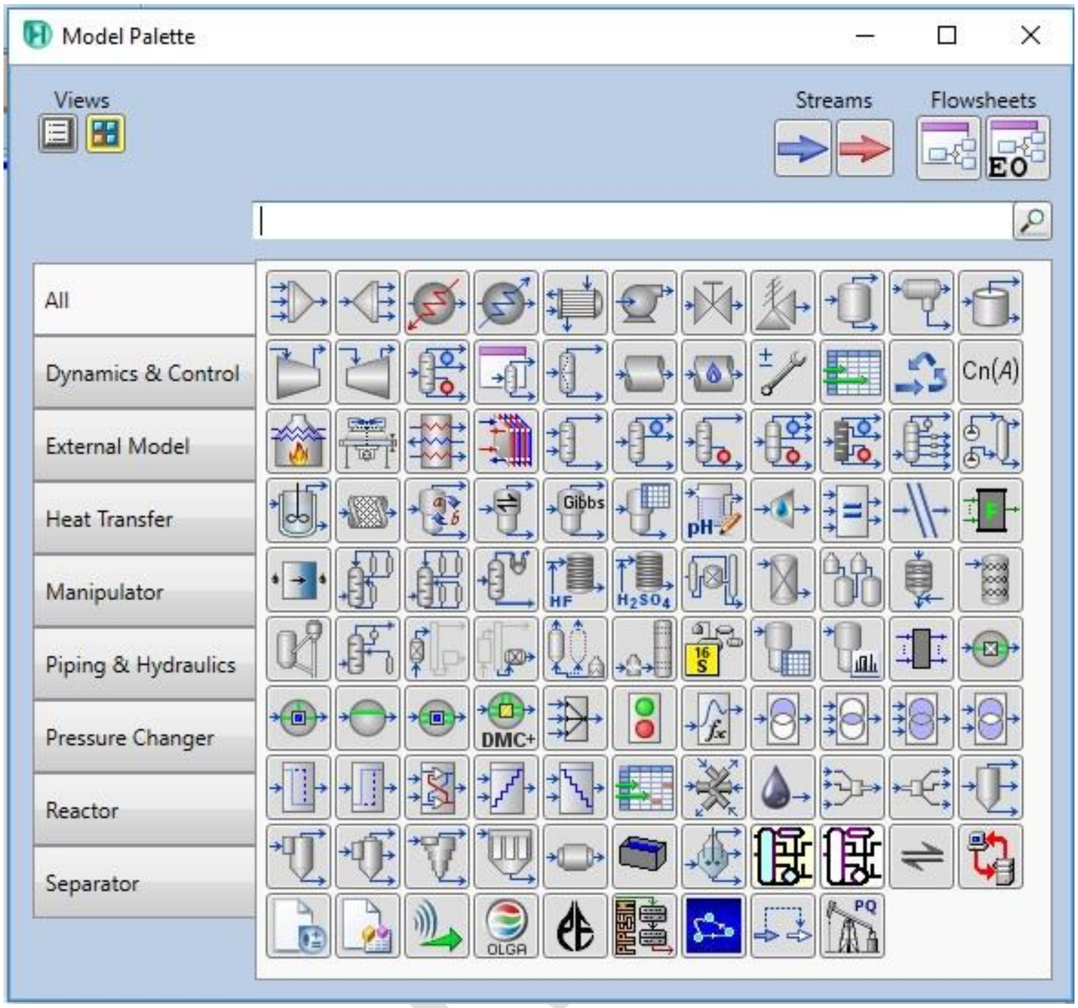

Figure 7. Palette of Different Devices in Aspen HYSYS

1-8-3- Thermodynamic Databases of Aspen Hysys

Thanks to its capabilities, Aspen Hysys can easily handle complex operations and processes due to its wide range of databases, which contain almost all known components (a large number of components). This gives the user the ability to select the necessary components for their simulation without relying on external resources. Therefore, Aspen Hysys is rich in data regarding different components, which can also be updated in available updates and the support center. Further information about the different resources adopted for Aspen's database can be found in the appendix table.

However, Aspen Hysys provides the user with the option to select different thermodynamic models to complete and determine various calculations during the simulation process. This process requires some knowledge about the different models (over 30 models) to make a selection that corresponds to the components used. More information on this part will be discussed in the next section.

1-8-4- Selection of the Appropriate Thermodynamic Model

Another key to successful simulation lies in selecting the most appropriate thermodynamic model based on the specific simulation and different conditions. This is primarily because each method available in Aspen Hysys is only suitable for particular types of components and limited to certain operating conditions. This fact underscores that choosing the wrong method can lead to incorrect simulation results; therefore, this step is truly important for reliable calculations associated with the desired operation (distillation, liquid-liquid extraction, etc.).

Consequently, to perform this step, several steps must be followed:

- Select the most appropriate thermal model/method according to recommendations.
- Compare the predictions obtained with literature data.
- Add estimations for components not available in the chosen thermo package.
- Generate laboratory data if necessary to verify the thermal model.

Moreover, several points must be considered when selecting the appropriate thermodynamic package, among which these stand out:

- Nature of the mixture (e.g., hydrocarbon, polar, electrolyte, etc.).
- Pressure and temperature range.
- Availability of data.

1-8-4-1- Recommendations for Selection of Thermodynamic Package

According to literature and shared engineering knowledge regarding simulation parameters using Aspen Hysys, there are three widely known recommendation references, which are:

- Eric Carlson, “Don’t gamble with physical properties for simulations,” Chem. Eng. Prog. October 1996, 35-46
- Prof J.D. (Bob) Seader, University of Utah
- Hyprotech Recommendations

Each of these recommendations is based on different problems presented earlier, where the selection of the most appropriate thermodynamic model directly depends on the properties of the components used in the simulation and associated parameters.

In summary, this chapter provides an in-depth overview of computer-aided design (CAD) and simulation, highlighting its significance in various engineering domains, particularly in chemical engineering. The chapter also introduces the Aspen Hysys software, discussing its features and usage in the simulation process. Further details on thermodynamic databases, selection of thermodynamic models, and recommendations for package selection have also been presented.

- **<u>Eric Carlson recommandations</u>**

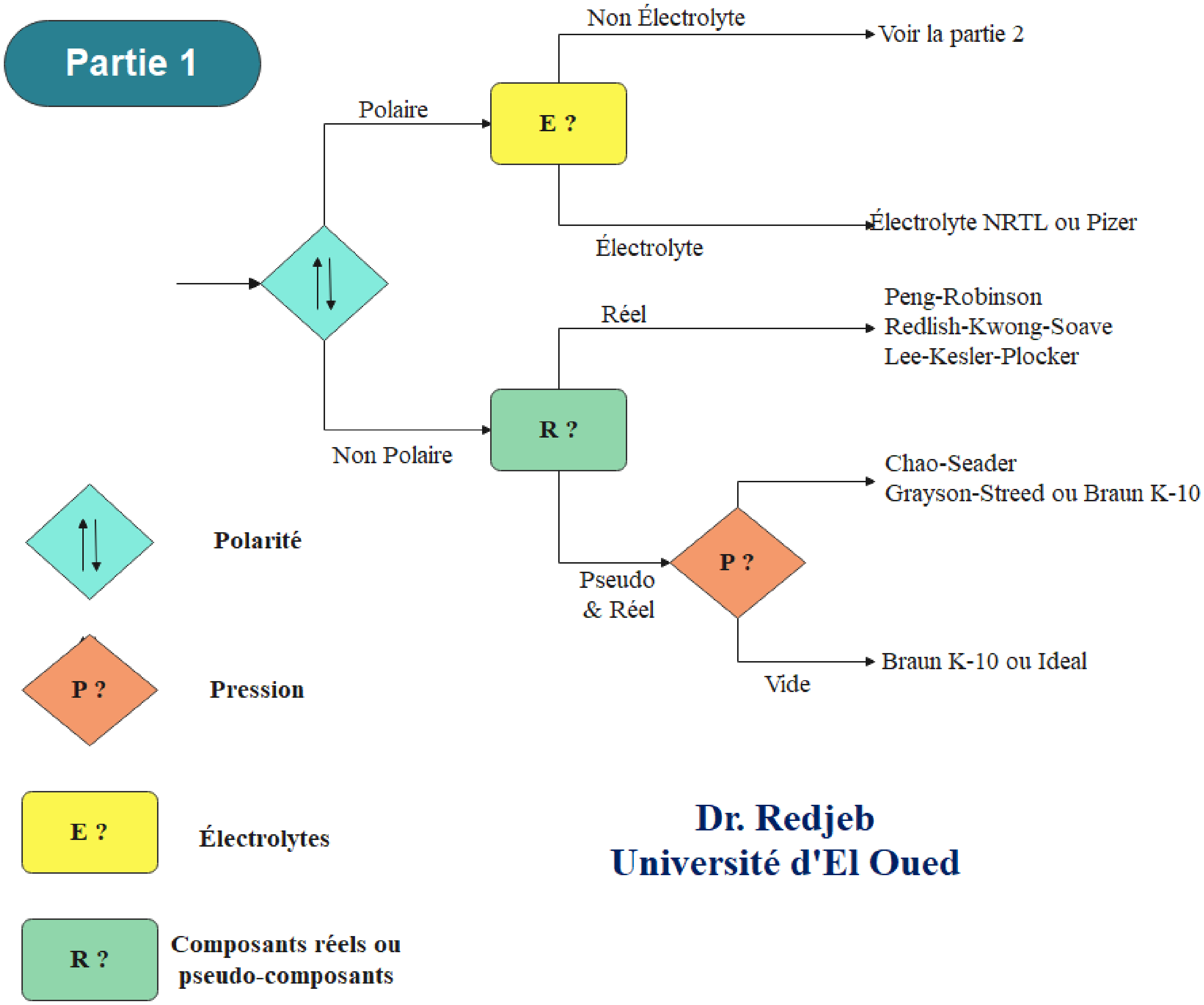

Figure 6. Eric Carlson recommandations part 01

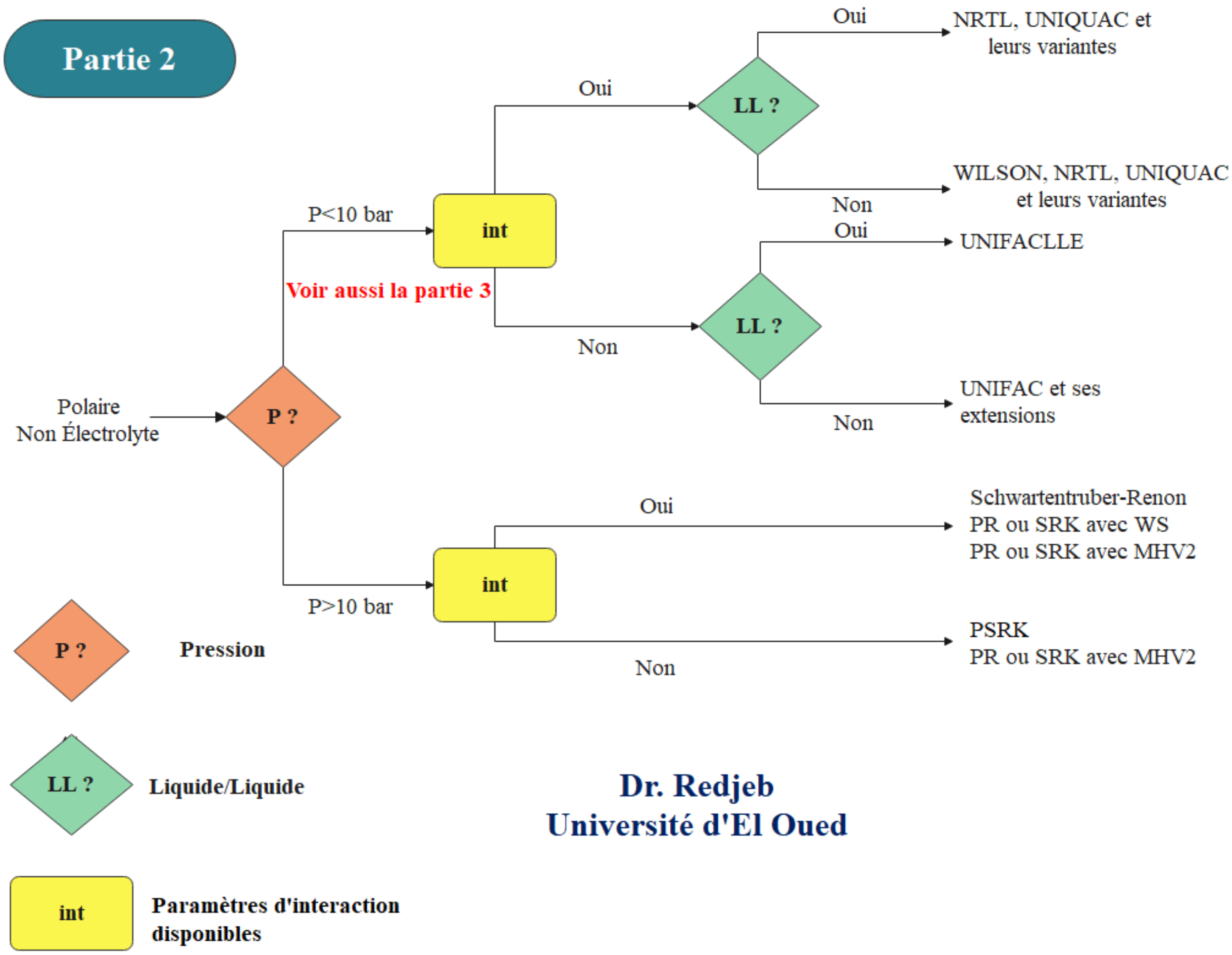

Figure 7. Eric Carlson recommandations part 02

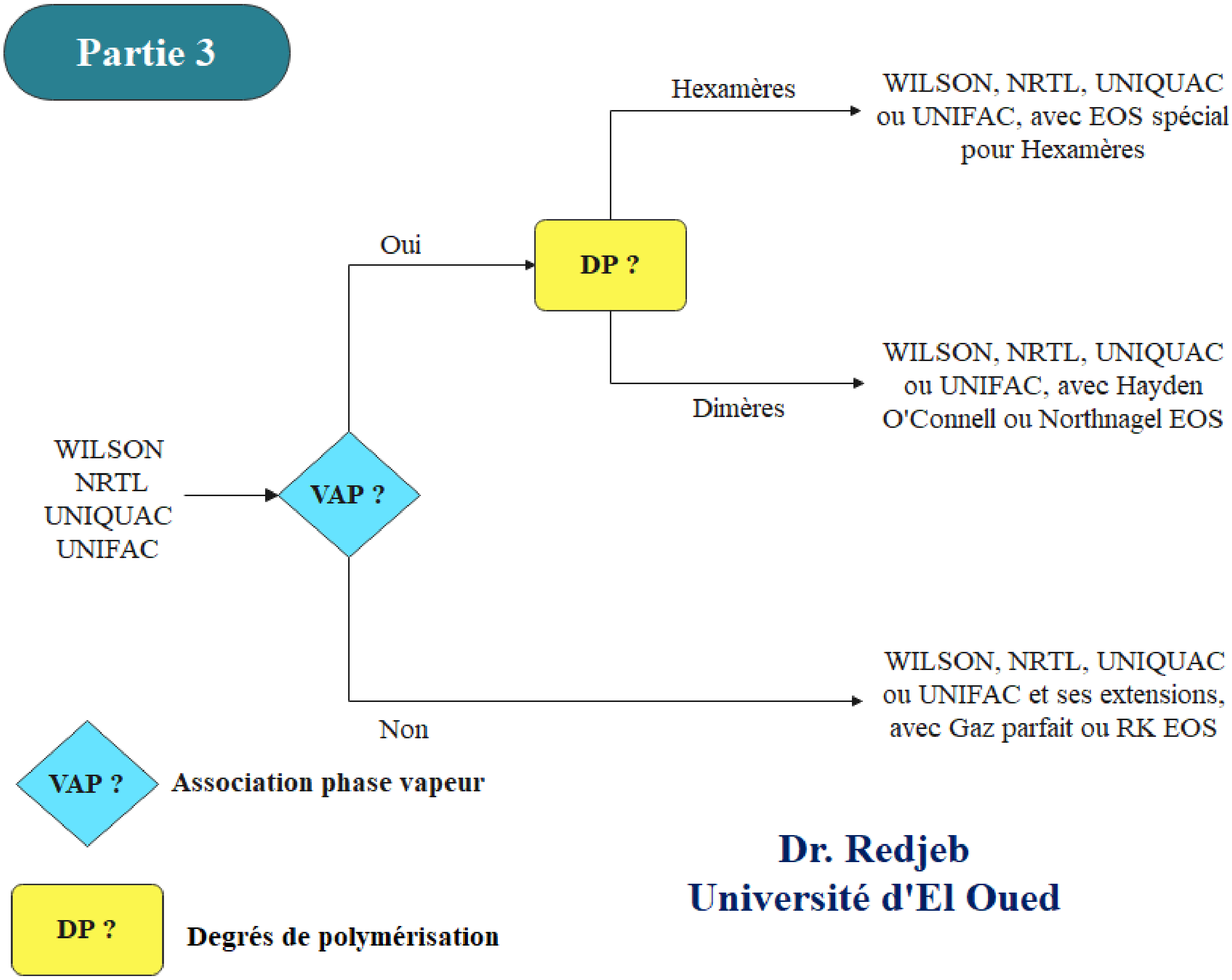

Figure 8. Eric Carlson recommandations part 03

- **<u>Bob Seader recommandations</u>**

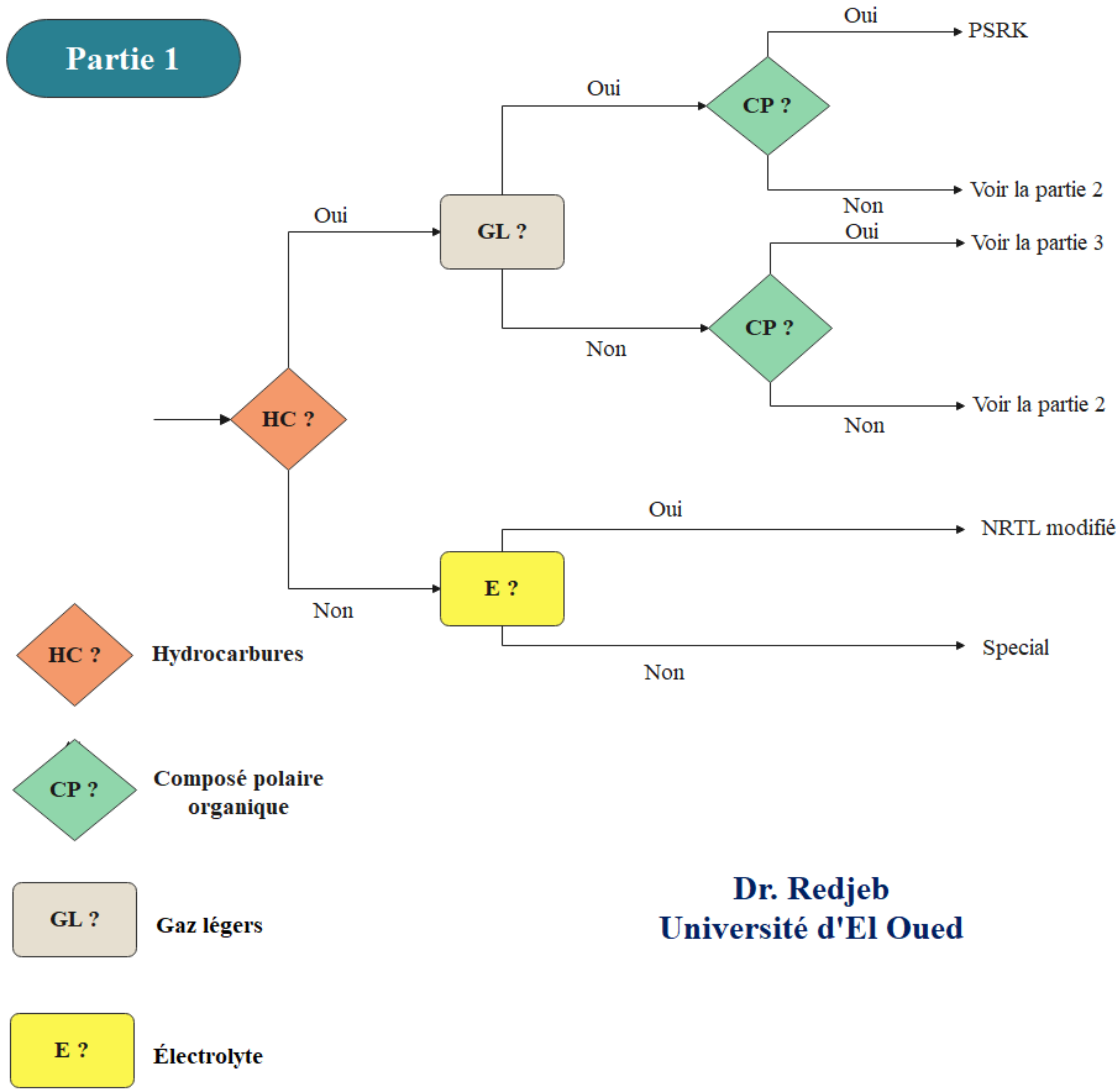

Figure 9. Bob Seader recommandations part 01

Partie 2

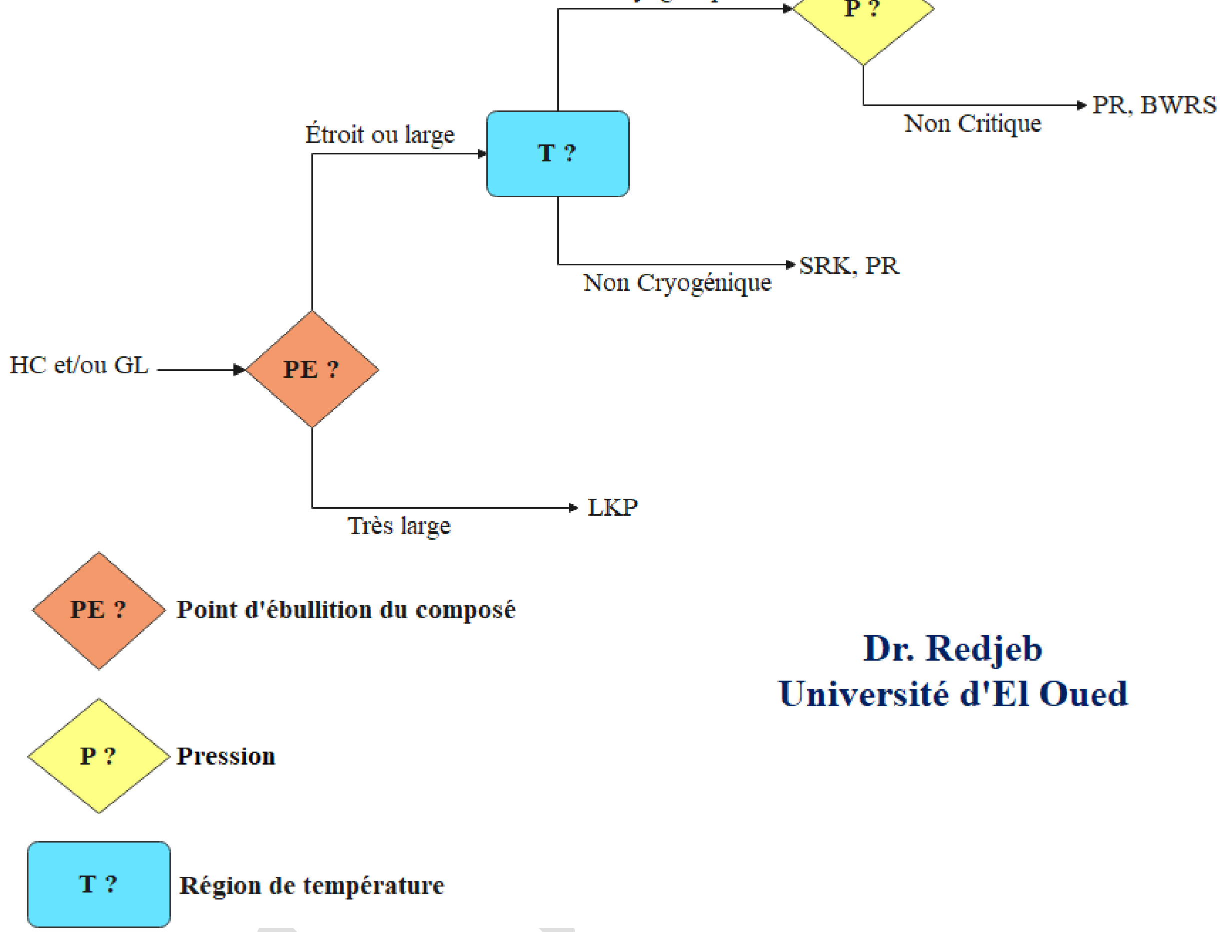

Figure 10. Bob Seader recommandations part 02

Partie 3

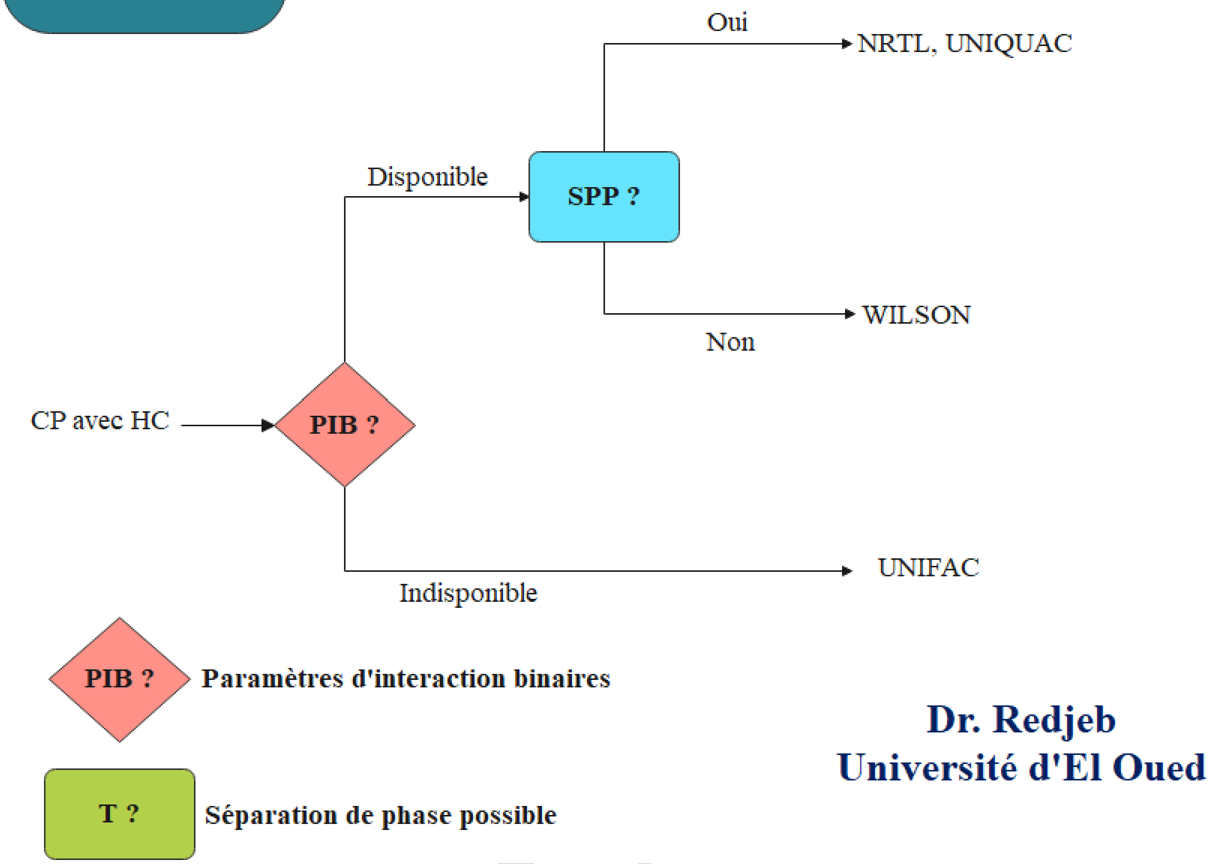

Figure 11. Bob Seader recommandations part 03

- **Hyprotech Recommendations**

Type of System	Recommended Property Method
TEG Dehydration	PR
Sour Water	PR, Sour PR
Cryogenic Gas Processing	PR, PRSV
Air Separation	PR, PRSV
Atm Crude Towers	PR, PR Options, GS
Vacuum Towers	PR, PR Options, GS (<10 mm Hg), Braun K10, Esso K
Ethylene Towers	Lee Kesler Plocker
High H2 Systems	PR, ZJ or GS (see T/P limits)
Reservoir Systems	PR, PR Options
Steam Systems	Steam Package, CS or GS
Hydrate Inhibition	PR
Chemical systems	Activity Models, PRSV
HF Alkylation	PRSV, NRTL (Contact Hyprotech)
TEG Dehydration with Aromatics	PR (Contact Hyprotech)
Hydrocarbon systems where H2O solubility in HC is important	Kabadi Danner
Systems with select gases and light hydrocarbons	MBWR

Figure 12. Hyprotech recommendations

Appendix 01

Table 01. Databases on ASPEN Physical Properties

Databank	Contains	Use
PURE32	Data from many sources, including DIPPR*, ASPEN, PCD, API, and Aspen Technology	Primary pure component databank in the Aspen Physical Property System
NIST-TRC	Data from the National Institute of Standards and Technology (NIST), Standard Reference Data Program (SRDP).	Data for a vast range of components. Available only with the Aspen Properties Enterprise Database.
AQUEOUS	Pure component parameters for ionic and molecular species in aqueous solution	Calculations containing electrolyte
ASPENPCD	Databank delivered with Aspen Plus 8.5-6	For upward compatibility
BIODISEL	Pure component parameters for components typically found in biodiesel production processes	Biodiesel processes
COMUST	Pure component parameters for components typically found in combustion products, including free radicals	High-temperature, gas phase calculations
ELECPURE	Pure component parameters for some components commonly found in amine processes	Amine processes
ETHYLENE	Pure component parameters for components typically found in ethylene processes for the SRK property method	Ethylene processes
FACTPCD	FACT species (components referenced in a specific pure or solution phase for use only with the Aspen/FACT/Chemapp interface in Aspen Plus)	Pyrometallurgical processes
HYSYS	Pure component and binary parameters needed by Aspen HYSYS property methods	Models using Aspen HYSYS property methods
INITIATO	Property parameters and thermal decomposition reaction rate parameters for polymer initiator species. Available in Aspen Polymers and Aspen Properties.	Polymer initiators
INORGANIC	Thermochemical properties for inorganic components in vapor, liquid, and solid states	Solids, electrolyte, and metallurgy applications
NRTL-SAC	Pure component parameter XYZE containing segment representations of common solvents	Calculations using NRTL-SAC property method
PC-SAFT, POLYPCSF	Pure and binary properties for PC-SAFT-based property methods.	Short hydrocarbons and common small molecules
POLYMER	Pure component parameters for polymer species. Available in Aspen Polymers and Aspen Properties.	Polymers
PPDS	Customer-installed PPDS databank. For customers who have licensed the PPDS databank from the National Engineering Laboratory (NEL).	Pure component data

Source: Aspen Plus R, www.aspentech.com

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