Modelling Thermo-chemical Hydrogen Generation in a Solar Plant

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Abstract: This article presents the work-in-progress of dynamic modelling works of hydrogen generation in Hydrosol3D project. This project has been based on the results of the Hydrosol II project where a pilot plant at the Plataforma Solar de Almería (CIEMAT) with the aim of producing continuously hydrogen was set up. The hydrogen is produced from water and concentrated solar radiation, based on a two step cycle process. In this process different chemical reactions occur, with an important dependence of the temperature inside the reactors. Several dynamic models for simulation and control system design are been developed currently and its progress is presented in this work-in-progress article. The mathematical models of the different subsystems are presented and first simulation results are commented.

Keywords: Dynamic Modelling, Object-Oriented Modelling, Modelica, Simulation, Hydrogen Production, Thermo-chemical, Solar Energy.

1. INTRODUCTION

The rise of the technologies related with the hydrogen has intensified the research of new ways of hydrogen production (Pregger et al., 2009). One of the most promising techniques to produce hydrogen is through two-steps redox systems in which at the first cycle (generation), a reduced metal oxide absorbs the oxygen of water producing hydrogen and at the second cycle (regeneration), the oxide is reduced again, releasing the absorbed oxygen at the water splitting. Since, these two reactions work at different temperatures, two reactors are required to produce continuous hydrogen flow rate.

At Hydrosol II project, the temperature in the reactors was controlled manually based on previous experiences and varying the number of heliostats focused on each reactor. For this purpose, the solar field was divided in different sections according to the flux contribution of each heliostat in the reactors (Roeb et al., 2011). One of the aims of HydroSol-3D project is the automation of the hydrogen production, including control algorithms to reach the desired temperatures in the reactors and follow the two step cycles. Moreover, the controller must be able to reject disturbances in irradiance to make viable the whole system. Therefore the first step is the development of realiable models for the generation process. These models will be used as a simulation tool to tune and test control algorithms.

2. SYSTEM DESCRIPTION

The pilot plant, set up at the Plataforma Solar de Almería (Roeb et al., 2011), consists in two reactors where the reactions associated to each cycle take place in parallel (Fig. 1). When the cycle ends, the reactions switch between the reactors. As a result, there is a continuous hydrogen production. For the reaction to take place, a controlled amount of power must arrive at the aperture of the receiver. This power comes from the heliostat field. Due to the different reaction rates of both cycles, the thermal power must be different in each cycle (Fig. 2). From a dynamic system point of view, the plant in Fig. 2 could be analyzed as follows. Each reactor receives only one inlet flow controlled by MV1 and MV2 valves. One inlet flow is N2 and the other H2O-N2. The N2 is heated up by H0 or H1 heater depending on the branch. The H2O-N2 mixed flow is heated up by H2 heater and it must be controlled in volume and in composition by FC2 and FC3 valves.

3. MATHEMATICAL MODEL

Modelica language (Modelica Association, 2007) is a model modeling language which allows an acausal formulation.
of the equations and an object-oriented programming. Formulating the problems in an acausal way makes easier to translate mathematical models in a formulation which Modelica can interpret avoiding the hard work of giving an explicit causality of all the equations. Object-oriented programming techniques may include features such as data abstraction, encapsulation, messaging, modularity, polymorphism and inheritance. These characteristics make save source code which allow reusing it in different modules.

Given the complexity of the model presented in this paper, the system has been divided in two parts, the heliostat field model and the process plant model which are also divided into other modules. In figure 5, the relationship between these models can be observed. The inputs of the heliostat field model are the solar irradiance and the heliostats in the field which are focused, and the output is the solar flux concentration. This flux is also the input of the process plant model; the other input is the mass flow and composition of the inlet gas. As outputs, the model has the reactor temperature, the gas temperature and the mass flow with its composition.

### 3.1 Heliostat Field flux model

One of the research lines, which have been carried out in the last years, is the development of reliable solar field models of central receivers to study the behavior and contribution of the solar fields. Several codes are available to calculate the solar flux concentration and its distribution on a central receiver system with a heliostat solar field. As it is explained in García et al. (2008), two categories may be distinguished regarding to flux calculation codes. The first one includes software to design solar plants to maximize the collected solar energy, whereas the second category includes codes for evaluating the power reflected by the heliostats and collected on the receiver. Since these codes are designed to obtain high degree of precision, the numerical models may be slow to be used in real-time applications. In Belhomme et al. (2009), a new software is included to calculate the flux density distribution reducing the computation time. Nevertheless, this time is still slow to be useful in real control applications.

So, a simplified model have been developed for this kind of real time applications, and a prediction of the whole mean concentrated solar radiation in each of both focus is predicted. To reduce the complexity of the model, it have been assumed that there is no slope and tracking errors, there is a homogeneous flux density on the receiver plane and the shading and blocking are assumed as constants.

Then, the flux concentration in the receiver, $F$, may be approximated as:

$$f_k = I \cdot \cos(\alpha_k) \cdot A_h \cdot \beta \cdot (1 - \gamma),$$  

$$F = \sum_{k=1}^{N_h} f_k$$

where $N_h$ is the number of heliostats in the field, $I$ is the direct solar irradiance, $\alpha_k$ is the solar vector incident angle in the heliostat plane, $A_h$ is the heliostat mirror area, $\beta$ is a parameter which includes slope and tracking errors and $\gamma$ is the atmospheric attenuation factor. To determine the coordinates of the Sun, the algorithm proposed in Blanco-Muriel et al. (2001) is used.

The Fig. 4 presents the first results of the simulation of this model using a Hydrosol-3D data as inputs. The flux which is concentrated in one receiver is computed depending on the incident irradiance, date, hour and the focused heliostats.

### 3.2 Process Plant model

In order to reduce the computational effort, the model presented in this subsection is a simplification of the real plant shown in Fig. 1. As in section 3.1, it is important to obtain a fast model in spite of reaching a lower degree of accuracy.

Due to the existence of multiple chemical species in the reactor, the object-oriented approach applied in the ThermoFluid library (Tummescheit, 2002) has been applied. The reactions implemented and its rates are defined in...
ThermoFluid provides a set of components that let model by inheritance and parameterization chemical reactions in gas phase. Three main components have been used:

- **GasMixHydrosolII.** Subclass of IdealGasMixProps, it is the medium used in the process and modeled as perfect mix of ideal gases. Six ideal gases are assumed in a perfect mix: H2O (superheated water steam), N2 (nitrogen), H2 (molecular hydrogen), O2 (oxygen), H (atomic hydrogen, representing a 'virtual gas specie' for coating Oxygen absorption), and OH ('virtual gas specie' for coating Oxygen generation).

- **Volume2PortS.** This class is a control volume which models mass and energy conservation for all the chemical species inside it, accounting for the multispecie flows in two connectors. In includes a replaceable reaction class parameter that let define custom reactions. It is parameterized for the medium previously defined.

- **Reaction.** This model lets define model for a reaction, in which basically the number of reactions and its rates have to be defined in a structured way. The dynamic evolution of the different products and reactants is modeled then.

Using this approach, the thermofluid behaviour of the process plant is extended with the modelling of the chemical species in the reactors, and the hydrogen production could be predicted. In the next section preliminar non calibrated simulation results are presented.

4. SIMULATION RESULTS

Due to the state of work-in-progress, the model does not predict with enough reliability the output concentrations but it predicts the thermal behavior with an important reliability degree. In fact, the chemical concentration components submodels are based on the thermal model, and its former development must be completed to begin with the chemical calibration and validation. During this year, experimental work is going to be performed at Plataforma Solar de Almería, that will let afford a more accurate calibration and validation, thermal and chemical submodels.
In Fig. 6 is shown a simulation of the model where the input power flux used is the same which was obtained in the simulation shown in Fig. 4.

Another simulation based in the thermo-chemical model of Fig. 5 is presented in Fig. 7, in which the H2 generation and regeneration needed temperatures are reached, by the focusing of concentrated solar power in each reactor. In the different cycles and at different temperatures, generation and regeneration are produced. Fig. 8 presents preliminary O2 and H2 concentration evolutions for each of the corresponding cycles.

Another simulation results of the presented model, working in closed loop with a PI controller is depicted in Fig. 9. These graphs show the variations in irradiance, number of heliostats which are focused, temperature in one reactor and the mean flux on the receiver. The setpoint in the temperature switches between the two typical temperatures used for regeneration and production (1473 K, 1073 K), whereas the flux setpoint switches between 45 kW and 15 kW (Roeb et al., 2009). This controller has been tuned so that the response obtained is slow but robust, avoiding overshoots in the reactor temperature. Nevertheless, the performance of the controller may be tuned varying the typical parameters of the PI controller and more advanced control techniques will be applied.

5. CONCLUSIONS AND ONGOING WORK

Several models for hydrogen solar production plant have been presented. They are based on first principles and it has been developed using the modelling language Modelica, an acausal and object oriented language. Inside Modelica, the ThermoFluid library for object oriented modelling of thermo-chemical phenomena has been used. The complete model has been divided into two modules, the heliostat field which predict the flux power concentration and the hydrogen generation process plant which predict the termo-chemical behavior of the plant. One main advantage of this model is its low computational effort which makes testing control algorithms more efficient. Furthermore, several simulations results have been presented, some of them using real input data real operating conditions. Although, more experiments are planned to be performed for an accurate calibration and validation of the
models. This experiments will be carried in the scope of EU financed Hydrosol-3D Project.

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