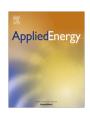
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# Unified modeling and feasibility study of novel green pathway of biomass to methanol/dimethylether



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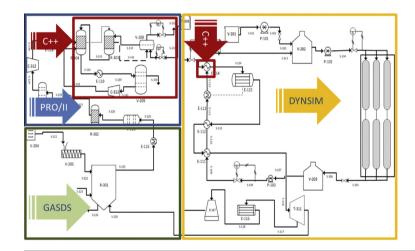
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#### HIGHLIGHTS

- Design, simulation, and control of the direct-storage concentrating solar plant.
- Feasibility study of the lowtemperature biomass gasification.
- First-principles model of biomass gasifier.
- First-principles model of one-step methanol/dimethylether synthesis reactor.
- Integrated numerical platform for total plant simulation.

#### $G\ R\ A\ P\ H\ I\ C\ A\ L\ A\ B\ S\ T\ R\ A\ C\ T$

Biomass-to-methanol/DME synthesis process layout.



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#### $A\ B\ S\ T\ R\ A\ C\ T$

A novel, integrated and unified process is proposed, modeled and studied for converting biomass to methanol (MeOH)/dimethylether (DME) to demonstrate its feasibility and applicability for the global industrial sector. The unified process consists of a concentrating solar power (CSP) plant, which supplies the produced steam to the biomass gasification process as well as to the downstream conversions to chemical commodities and energy carriers. To preserve the effectiveness of the biomass gasification with low-temperature solar-powered generated steam (approximately 400–410 °C), the gasification process is studied by means of a multi-complex (multi-scale, multi-phase, and multi-component) model and adapted to the novel proposed conditions. The syngas generated in the biomass gasification unit is then converted into MeOH/DME by means of one-step synthesis technology to improve the overall yield of the biomass-to-methanol process.

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#### 1. Introduction

Process integration is generally defined as being related to the process design to emphasize the unity of the process and interaction between different unit operations, or different plants in operation, in order to employ the resources effectively and

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minimizing the costs and energy consumption throughout the process [1-3]. Considering the environmental concerns to meet the free emission approaches is another significant motivation of the process integration, which is accomplished not only designing new facilities and process layouts, but also replacing some traditional resources by new and greener one [4–7]. From this perspective, it would be synergistic to provide the combination of the various energy sources, renewable and non-renewable sources, and process engineering is unavoidably the key-step in combining and integrating sources in a sustainable way with an additional advantages for the energy sector and industries [6]. The generation of clean and emission free source of power for facilities plays a key role in the sustainability of the processes and, as it is understandable, the dependency of the chemical industries on the steam availability falls into this element [8,9]. It is therefore promising to provide an alternative for the clean production of steam rather than traditional and common technologies, which are complex, highly sophisticated and expensive processes [9]. Traditionally, power plants are based on coal-fired power/steam generation. All conventional sources of steam generation such as gas turbine combined cycle (CC) [10,11], integrated gasification combined cycle (IGCC) [12–14], and pressurized fluidized bed combustion (PFBC) [15,16] are fuel based steam generation processes [8]. Environmentally speaking, decreasing the carbon footprint in chemical plants requires the intensive attempts to optimize the energy requirements by reduction of the consumption of the energy and lessen the carbon emissions associated with the remaining energy. The idea of shifting the energy resources of chemical plants to renewables such as solar and wind is reinforced if appropriate storage technologies are developed [6] to make continuous the power supply that comes from a discontinuous source. The concentrating solar power (CSP) plant is suggestively an attractive opportunity for power generation considering it as the source of energy without carbon footprint, and performing in a form of electricity or steam. It might be claimed that the CSP plant is a unique renewable resource of power generation, which can easily be coupled with other units to operate only by the means of thermal energy storage (TES) to make it highly dispatchable throughout the process [17.18]. However, it becomes more complex for research investigation relying on modeling and simulation tools due to the lack of reliable models and appropriate accessible simulators to model the renewables and demonstrate the feasibility of such facilities. The complexity is found especially when the simulation is required for the entire plant, which includes the integration of non-conventional units, complex and non-ideal thermodynamic data and libraries, innovative equipment and uncommon components for the process operations. Many of the above elements are not included in the commercial packages for process modeling, typically addressed to the oil and gas and process industry [19], and have to be developed ex novo and integrated and synchronized in these packages. Although, few dynamic modeling and simulations were performed to improve the knowledge and the effectiveness of solar plants facing design [20], numerical simulation [21], economic issues [22] monitoring [23], prediction [24] and control [25] of the thermal energy storage methods, they are still not based on well-established commercial dynamic simulators. In investigating the reason, it is evident that these types of plants contain operating units (i.e., the solar collector) deeply dissimilar to the conventional units adopted elsewhere [26] and traditionally included in the model library for process simulations such as AspenHysys and Pro/II. Therefore, it would be possible to either provide a new model or transforming the existing models to search for a reasonable accuracy for the simulation. Some issues for the CSP plant simulation have been already faced by the authors in prior works [18,27], mainly dealing with the heat exchange train for steam generation from hot molten salt streams.

Unavailability of mathematical models is one of the main issue making stiff the studies of novel process layouts that want to integrate renewable sources in the flowsheeting procedure and economical process assessments as well as slowing the advances in process engineering [18,19].

About the gasification process, it is obvious that although the reserves of coal are abundant and widespread geographically over the world [28,29], due to the price in comparison with oil [30–32] and also, the environmental issues competitive with biomass, it is not well allocated in the emission free and inexpensive category of feedstock for the energy sector [33,34]. Relying on addressed reasons, the focus on biomass was and is concentrating severely rather than coal and activities are driven toward bio-products, chemical commodities and bio-fuels in the near future starting from second, but also third, generation biomass. The Horizon 2020 program of the European Community is a clear example of this energy roadmap. Furthermore, biomass promises to provide the sustainability as a renewable feedstock. Following these approaches, replacing fuel-based power plants with renewable and clean sources of energy could bring benefits in comparison with the traditional ways of steam generation processes. Although several works have been accomplished in the gasification modeling and kinetics development [35,36], design of the gasifier [37,38] and effective operating conditions [39–42], no significant work is found on low-temperature biomass gasification in the literatures, which is the typical condition of the solar-powered steam generation taken into consideration in this work. The practical feasibility of the proposed low-temperature biomass gasification process is therefore investigated. The gasification unit has the ability to become an important and key facility in the energy and chemical process industry [43]. Coupled with this, nowadays, methanol is advocated to substitute oil and dimethylether (DME) as substitute natural gas [44], both of which are predominantly produced by steam reforming of methane (natural gas) and subsequent synthesis reactions of the produced syngas to methanol and, then, to DME. However, any source of organic material could be converted into syngas and so, methanol. Therefore, biomass from organic urban/industrial/ agricultural waste as feedstock could become a source of methanol in the near future [43,45-49].

Since the introduction of the high-pressure methanol synthesis in the 1920s, several technologies have been introduced to achieve low-pressure synthesis [50]. Nowadays, Lurgi, Haldor Topsøe and Davy Process Technologies allows to produce methanol at 60-100 bar from syngas (CO and H<sub>2</sub> mixture), which is usually obtained by means of steam reforming operations [44]. The methanol synthesis reactor is usually based on two fixed-bed tubular sections [51-54], a gas-cooled and a water-cooled section, although several other configurations have been proposed [43,55,56]. This paper is aimed at discussing the methanol/DME synthesis fed by the syngas produced in the biomass gasification process. The socalled one-step technology for the co-current production of methanol and DME is considered. It must be evoked that H<sub>2</sub>:CO ratio for methanol synthesis could be adjusted either in situ, where the reverse water gas shift reaction is active on the catalyst or using an ad hoc water gas shift reactor.

An overview of the unified plant of biomass-to-methanol/DME together with the tools adopted for the study is given in Section 2; CSP plant and TES are described and modeled in Section 3; biomass gasification process is characterized, designed, and simulated in Section 4; the one-step technology for methanol/DME production is deepened in Section 5.

#### 2. Overview of the unified plant and tools adopted

The main issues in modeling and studying the practical feasibility of a novel solar-driven route from biomass to MeOH/DME

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