Modelling Tar Conversion in a Partial Oxidation Reactor Using Flamelet Generated Manifolds

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Motivation

The amount of fossil fuels on planet earth is diminishing, while its consumption increases rapidly [1]. To ensure our energy supply, a gradual transition to other energy sources is needed. Renewable energy may play a significant role in this transition, with its additional advantage of being carbon dioxide neutral. Several technologies have been developed, including windmills and solar cells. However, the problem with these technologies is the storage of the produced electricity. The solution for this problem may lie in the transformation of electricity into chemistry: Power-to-Gas [2]. In Delfzijl (Groningen, NL) the first large scale, completely integrated Power-to-Gas installation will be build, in which green power is converted into hydrogen and pure oxygen via electrolysis. As schematically shown in figure 1, the produced hydrogen can be used as a raw material for the chemical industry. The pure oxygen can be used to gasify torrefied biomass into syngas; a valuable source for the chemical industry mainly consisting of carbon monoxide and hydrogen.

Figure 1: Schematic representation of the Power-to-Gas principle.

The gasification from biomass into syngas occurs in two stages: first torrefied biomass is converted under influence of heat into gas in a pyrolysis unit, and afterwards the arisen gasses are partially oxidized in a partial oxidation reactor, which will be developed by the A. de Jong Group. These gasification processes have been extensively investigated [3][4], and the major problem is the formation of tars in the pyrolysis unit. Tar is very easy to condense and difficult to remove, causing fouling in downstream processes. Several methods have been developed to reduce the tar content in syngas, including thermal conversion, catalytic cracking, mechanical separation and partial oxidation. It has been proven that partial oxidation can reduce the tar content significantly [5]. In this process, tars and other volatiles are partly oxidized, while the released heat is used for thermal cracking of the remaining pollutants. In this way, tar content can be reduced and converted into non-condensable gasses.

However, the elementary processes occurring at partial oxidation are not yet fully understood, and research is needed to ensure a satisfying tar conversion rate. Therefore, a 500 kW pilot plant has been built in order to verify the working principle of biomass gasification in a two-stage gasifier. However, satisfactory experimental results on a pilot plant is no guarantee for equal results on a full-scale installation. Therefore, experimental data from this pilot plant can be used to validate the modelling of tar conversion. When validated, numerical models can be used to predict tar conversion on a full-scale installation. Hence, the purpose of this study is to validate a numerical model on tar conversion in the pilot version of the partial oxidation reactor in order to predict tar conversion on a full-scale installation.

Method

Experiments on the pilot plant will be conducted according to the Design Of Experiments (DOE) principle, where measurement points are selected carefully by varying relevant factors simultaneously. These factors should be controllable, and chosen prior to the experiments. In tar conversion, temperature and residence time are of great importance [5]. In the two-stage gasifier, there are two important temperatures: the pyrolysis and partial oxidation temperature; the temperature of the pyrolysis reactor determines the amount
and composition of tars that have to be destructed under influence of the partial oxidation temperature. Both temperatures are measured, and can be controlled by varying the mass flow of oxygen into the reactors. Thus, these temperatures can be chosen as factors. The residence time determines the period for the tars to be subjected to these temperatures, and can be controlled via the mass flow of biomass through the system. Since the actual residence time is not measured, the mass flow of biomass is chosen as a factor.

As can be seen in figure 2, the measurement points are distributed in a cubic design space. On the axes the factors can be found, and in the middle of the cube there are three center measurement points to verify the reproducibility of the experiment. This approach enables the ability to map tar conversion as a function of the three chosen factors. A statistical model can be derived, and this model can be compared to numerical modelling results.

To obtain numerical tar conversion data, a three-dimensional model will be constructed in ANSYS Fluent. Since tar includes many species with different behaviour, an extensive reaction mechanism is needed to describe their formation and destruction. The reaction mechanism of Ranzi, consisting of 185 species and 6445 reactions, has been proven to predict tar conversion quite well [6]. So, this mechanism is chosen to describe the elementary processes. Since it is too extensive for direct integration, the Flamelet Generated Manifolds (FGM) reduction technique is used. In this approach, prior to the combustion simulation, a database of thermochemical variables (manifold) is generated as a function of control variables for given initial conditions. During run-time of ANSYS Fluent the transport equations for these control variables are solved, together with the momentum equations. All relevant combustion data can be retrieved from the pre-determined manifold, which reduces computation time significantly [7]. By simulating the same measurement points in a numerical model, a similar statistical model can be derived. Then, trends from the experimental and numerical modelling results can be compared, and conclusion can be drawn on the ability to model tar conversion in a partial oxidation reactor.

Results

Since experimental data is not yet available, results will not be presented.

References


