Entrained flow gasification: mathematical modelling based on RANS for design and scale-up

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Abstract

Production of synthetic fuels and chemicals in a closed carbon cycle economy is one of the main challenges concerning climate change. In order to convert biomass residues to high-density fuels, the bioliq® process [1] has been realised at Karlsruhe Institute of Technology (KIT). Between 2005 and 2013, all stages of the process were developed and commissioned including the bioliq entrained flow gasifier (bioliq EFG) [2]. During the design phase in 2008/2009, a basic numerical model of the bioliq EFG was already developed [3, 4] and its major limitations were identified. These include simplified sub-models for atomisation, for conversion of char, pyrolysis oil and suspensions thereof, for gas and particle radiation and for slagging at high-pressure and high-temperature conditions. Since 2013, many experimental bioliq EFG campaigns have been carried out and reliable experimental results have been obtained. In parallel, the work on the numerical model of the bioliq EFG has been resumed. This paper focusses on the status quo of the numerical model, on the accuracy of recent numerical results and on the challenges faced in the development of a CFD based tool for design and scale-up.

The numerical model is based on the RANS and the Euler-Lagrange approaches and assumes a steady-state. The rates of the gas-phase reactions are described either using the eddy-dissipation-concept model in combination with a reaction mechanism or using a relaxation-to-chemical-equilibrium model. Gas radiation is calculated using the discrete ordinates model and a weighted-sum-of-grey-gas model. The latter assumes six gases (five grey gases and one clear gas) and has been obtained from accurate line-by-line calculations. Slagging is implemented as boundary condition assuming both the downwards axial slag flow and the radial heat flow through the slag layer as one-dimensional. Temperature profiles in the liquid and the solid slag layer and in the wall are predefined as linear.

The numerical results are reported for the bioliq EFG experiment V82.1 in which a model fuel (96 % ethylene glycol + 4 % A-glass) was applied. The results show that both the total heat extracted from the bioliq EFG and the gas-phase composition at outlet can be predicted with good accuracy. Due to uncertainties in the prediction of particle deposition, some deviations are observed concerning both the local heat extracted by the six cooling segments and the slag thickness. Sensitivity studies show that simplifications of the gas-phase reactions are acceptable.

Introduction

Entrained flow gasification of biomass has the objective to produce green synthesis gas. Contrary to entrained flow gasification of coal, the biomass based process is currently on the pilot-scale level (TRL 6/7) and further scale-up requires appropriate models and validation results. Apart from the CHEMREC PEHT-BLG for the gasification of black liquor at the Energy Technology Centre in Piteå [5], the bioliq EFG has been realised at Karlsruhe Institute of Technology for the gasification of pyrolysis oil slurries. The bioliq EFG is the second stage of the bioliq® process [1] built-up and commissioned between 2005 and 2013. The design of the bioliq EFG was particularly based on numerous CFD studies carried out by Mancini et al. [3, 4] in 2008/2009. Several geometries and operating conditions were examined using a CFD model, and many sub-processes were simplified. The latter include atomisation, vaporisation,

decomposition, devolatilisation, homogeneous and heterogeneous gasification, ash transformation, radiation and slagging. Since 2011, several sub-processes have been investigated and sub-models have been improved. In thermal radiation, for example, absorption coefficients depend on wavelength, temperature, pressure and composition, and radiation at high-temperature and high-pressure conditions has to be taken into account appropriately. However, default line-by-line models or the emissivity charts of Hottel et al. [6, 7, 8] are known to be inaccurate for high-temperature and high-pressure conditions. Therefore, Alberti et al. [9, 10] revised the emissivity charts after introducing new cut-off criteria for line-by-line calculations using the current HITEMP-2010 database [11]. Emissivity charts can also be applied for weighted-sum-of-grey gas models [12], which are still a good choice for accurate and computational efficient radiation simulations.

Slagging is another aspect that was simplified in the design simulations. Mancini et al. [3, 4] applied a constant temperature as wall boundary condition for the energy equation in accordance with other CFD studies at that time. For example, Chen et al. [13, 14] used three different measurement-based temperatures as boundary conditions for the combustor, the diffuser and the reductor of the Mitsubishi Heavy Industries Entrained Flow Gasifier. Marklund et al. [15, 16] and Carlsson et al. [17, 18] applied a total heat flux estimated from measurements for the CFD model of the CHEMREC PEHT-BLG. In addition to temperatures and heat fluxes, slag flow models were suggested for wall boundary conditions. In 1998, Seggiani [19] proposed a simplified slag-flow model for CFD applications based on the studies of Reid and Cohen [20, 21]. Further studies of Benyon [22] and Bockelie [23] showed the beneficial potential of slag-flow models in CFD simulations. However, none of the slag flow models, as those proposed by Seggiani [19] or later by Yong et al. [24, 25], have been validated yet, and the extent of the beneficial potential is unclear.

In order to reduce the uncertainties emphasised above, combined experimental and theoretical research has been carried out in the frame of the research programmes of the Helmholtz Association of German Research Centres and in the frame of the Helmholtz Virtual Institute of Gasification Technology [26] to develop an improved mathematical model for design and scale-up. This paper reports on the status quo of the development.

Experiments

The bioliq EFG is equipped with a segmental cooling screen and operates mainly at 40 bar with a fuel input of 5 MW [2]. The bioliq EFG experiment V82.1 that is focused in this paper is based on a model fuel consisting of 96 % ethylene glycol + 4 % A-glass; ethylene glycol and A-glass have been used as surrogates for pyrolysis oil and straw ash, respectively. Since the SiC refractory was renewed before the experiment, it can be guaranteed that there have not been any previous solidified slag deposits on the cooling screen, which might have influenced the slag flow during the experiment. After the experiment, the bioliq EFG was shut down and slag thicknesses were measured at several positions inside the cooling screen.

In addition to measurements of slag thicknesses, flow rates of inlet streams, temperatures inside the refractory and of the cooling water and the gas-phase composition after the quench have been continuously monitored and recorded. Heat removed from the bioliq EFG, equilibrium and balance temperatures as well gas-phase compositions at the outlet of the bioliq EFG have been consolidated using an ASPEN flowsheet model. Further details are given by Santo et al. [27].

Mathematical model basis

The mathematical model is based on the RANS and the Euler-Lagrange approaches and a two-dimensional axis-symmetric geometry of the bioliq EFG. The Euler approach is used for the gas phase consisting of CH_4, $C_2H_6O_2$, CO, CO_2, H_2, H_2O, O_2 and N_2. Turbulence and vaporisation are described by the standard k-ε model and the classical vaporisation-diffusion model, respectively. Rates of homogeneous reactions are based on the eddy-dissipation-concept model combined with a global reaction mechanism, the HVI1 mechanism [28]. Heterogeneous reactions with respect to mineral matter transformation or soot formation are neglected. Slagging is implemented as boundary condition based on Seggiani [19]. The slag flow model assumes a one-dimensional downwards axial slag flow, a one-dimensional radial heat flow through the slag layer and linear temperature profiles in the solid and the liquid slag layer and in the wall.

Radiation is accounted for by the discrete ordinates model which is applied for five grey gases and one clear gas and uses the weight functions and the pressure-based absorption coefficients of a tailored weighted-sum-of-grey-gas (WSGG) model, which was generated for a well-defined gas-phase condition. The WSGG model is defined by

$$\varepsilon = \sum w_k(T)\ (1 - \exp(-a_k\ p_a\ L)), \tag{1}$$

where w_k and a_K are the weight and the pressure-based absorption coefficient of grey gas k, respectively. L is the path length and p_a is the partial pressure of the absorbing gases. The weight functions and the pressure-based absorption coefficients were obtained using line-by-line calculations (with the cut-off criteria of Alberti et al. [9, 10]) and using an emissivity chart for pressure path lengths between 0.001 bar cm and 6000 bar cm.

Results

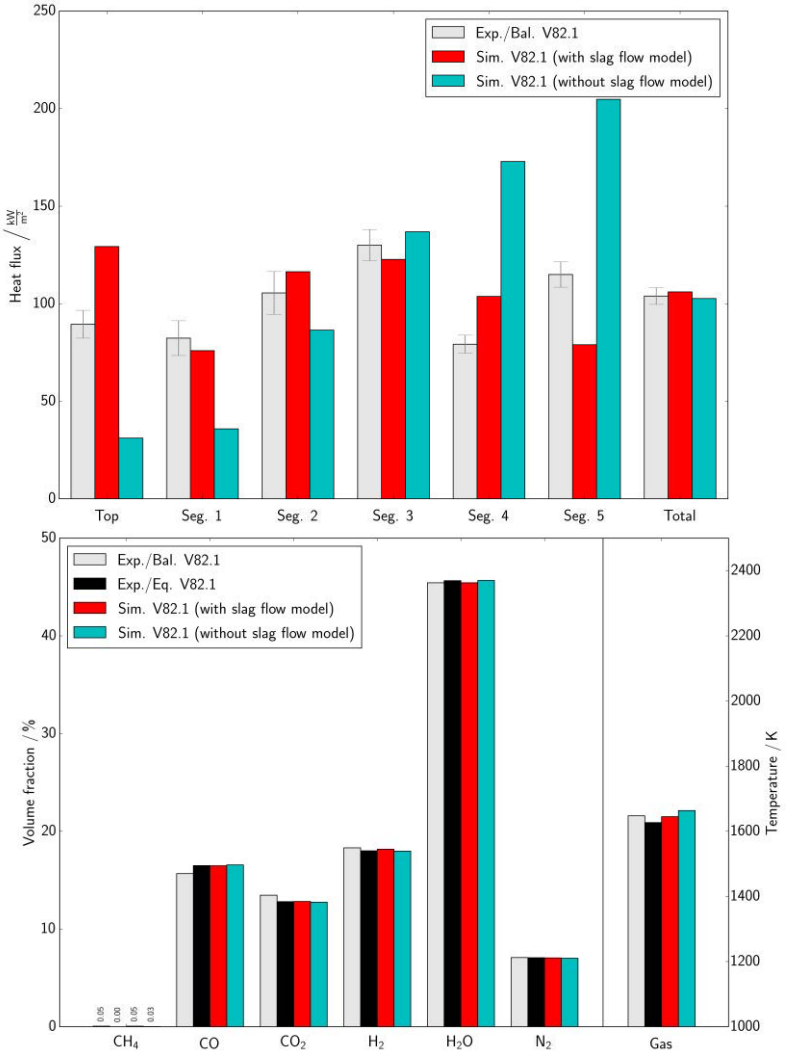

Figure 1. Comparison of the experimental and numerical results of the bioliq EFG experiment V82.1 concerning the segmental and total heat fluxes (top) and the gas-phase composition and the gas-phase temperature at outlet (bottom). *Exp./Bal.*: results based on measurements and balances [27]. *Exp./Eq.*: results based on measurements and equilibrium calculations [27]. *Sim.*: results based on CFD simulations.

In Fig. 1, the numerical results of the bioliq EFG experiment V82.1 are compared with the experimental results reported by Santo et al. [27]. While the gas-phase composition, the gas-phase temperature and

the total heat flux can already be predicted well with an appropriate boundary temperature, i.e. without a slag flow model, deviations in local heat fluxes are obvious for the segments. Those can be reduced by the use of a slag flow model. Particularly, the heat fluxes at the top and of the segments 1, 2, 4 and 5 show smaller deviations from the experimental results when slag flow is accounted for. However, some deviations still exist for the top and the segments 4 and 5, mainly due to imperfections of the near-boundary particle-tracking. Slag particles in the simulation impact on the refractory and deposit mainly in the lower part of the bioliq EFG. Only a few particles hit the refractory in the upper part while visual observations after the experiment show a uniform slag layer.

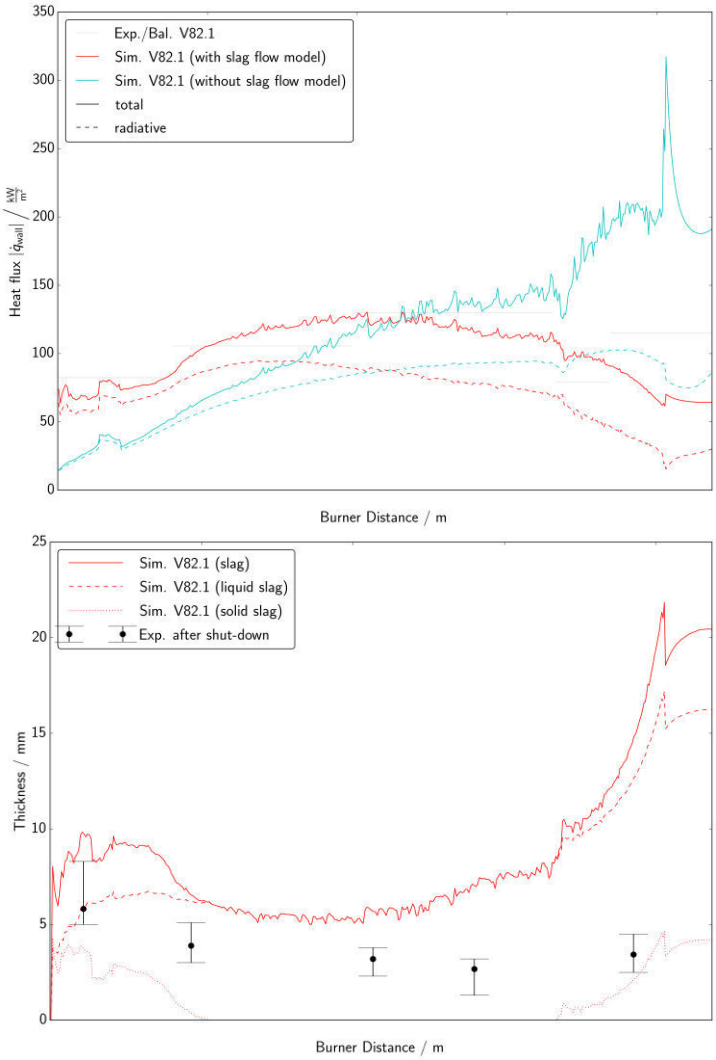

Figure 2. Comparison of the experimental and numerical results of the bioliq EFG experiment V82.1 concerning the local wall heat fluxes (top) and the slag thickness (bottom). *Exp./Bal.*: results based on measurements and balances [27]. *Exp. after shut-down.*: results based on measurements after the experiment. *Sim.:* results based on CFD simulations.

In Fig. 2, the predictions of both the total (convective and radiative) heat fluxes and the radiative heat fluxes along the burner distance, i.e. the bioliq EFG axis, are depicted. While the curve of the total heat flux underlines the results shown in Fig. 1, the curve of the radiative heat flux emphasises the significance of radiation, which amounts to 40 % to 95 % of the total heat flux. Fig. 2 also depicts the solid, the liquid and the total slag thicknesses along the burner distance predicted and the slag thicknesses measured. In the upper part of the bioliq EFG, the predictions are in good agreement with observations. Unfortunately, this does not apply for the lower part. In addition to the particle-tracking inaccuracies, the comparison of measured and calculated slag thicknesses is restricted through the slag

flow behaviour during the shut-down. Preliminary results of transient and simplified slag flow simulations using estimated temperature profiles indicate that some slag from the central and the lower part of the bioliq EFG might have flowed down the cooling screen during the shut-down. The slag layer in the upper part is less affected.

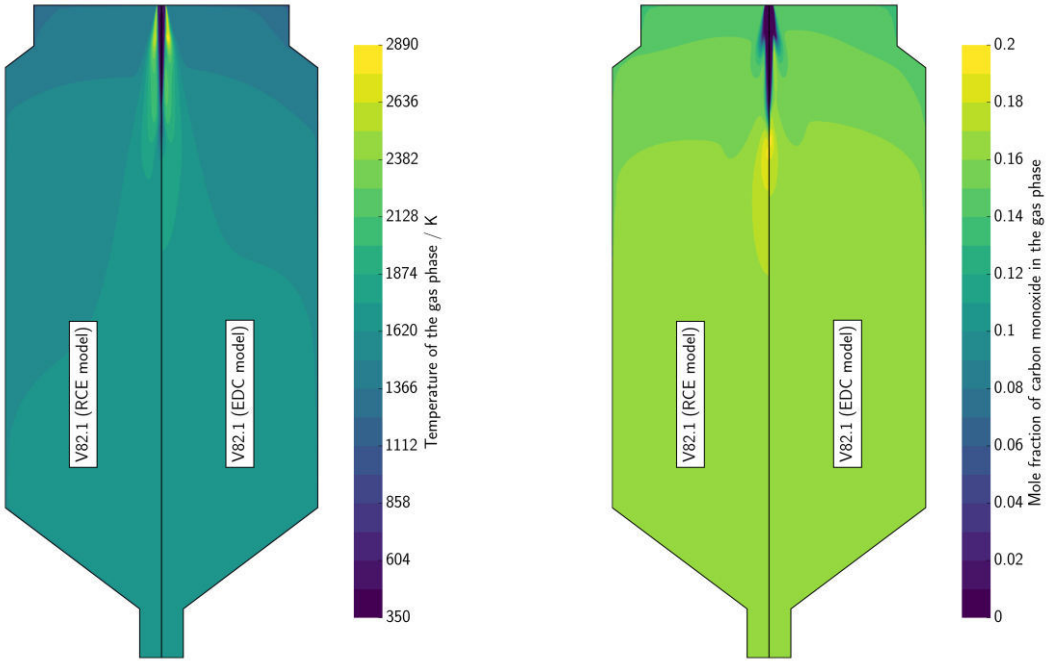

Figure 3. Comparison of the distributions (not to scale) of the gas-phase temperature (left) and of the gas-phase mole fraction of carbon monoxide (right) for the bioliq EFG experiment V82.1: influences of the turbulence-chemistry interaction model (relaxation-to-chemical-equilibrium (RCE) model vs. eddy-dissipation-concept (EDC) model).

In order to access sub-models uncertainties, a sensitivity analysis has been carried out. For example, a simplified chemistry model was applied instead of the eddy-dissipation-concept model in combination with the HVI1 mechanism. This simplified chemistry model is based on a relaxation-to-chemical-equilibrium approach predicting the equilibrium composition after long residence times. Fig. 3 compares the gas-phase temperature distributions and the gas-phase mole fraction distributions of carbon monoxide for the two chemistry sub-models. Slight differences can be observed in the upper part only. The simplified chemistry model decreased the flame temperatures and reduced the maximum temperature from 2885 K to 2630 K. The far-flame temperatures increased slightly resulting in an increased heat removal in the upper part. Apart from that, similar gas-phase temperature and gas-phase mole fraction distributions have been obtained since the bioliq EFG experiment has been designed to operate at gasification stoichiometry corresponding to a high adiabatic temperature. Therefore, it is not too surprising that the differences between the predictions obtained using the above chemistry models are small. At such conditions, equilibrium states can be reached fast and, thus, simplified chemistry can definitely be used.

Conclusions

Numerical simulations of the bioliq EFG experiment V82.1 were carried out, in which a model fuel consisting of 96 % ethylene glycol + 4 % A-glass was supplied to the bioliq EFG operating at 5 MW fuel input and at 40 bar. The numerical results were in good agreement with the experimental results concerning the overall performance of the bioliq EFG since the gas-phase temperature and the gas-phase composition at outlet were very well predicted. The implementation of a slag flow model improved the heat-transfer predictions although some deviations are still present due to inappropriate near-boundary particle tracking. While this requires further research and advanced sub-models, simplified sub-models

might be an option for other aspects as the comparison of two chemistry sub-models has shown. Predictions using the relaxation-to-chemical-equilibrium model and using the eddy-dissipation-concept model combined with a global reaction mechanism were only marginally different from each other. If experiments are thus designed based on high adiabatic temperatures, simplified chemistry can be applied in the overall model.

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