

ENTRAINED FLOW GASIFICATION: EXPERIMENTS AND MATHEMATICAL MODELLING BASED ON RANS

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Abstract

Interdisciplinary research has been conducted in the frame of the Helmholtz Virtual Institute for Gasification Technology (HVIGasTech) [1-4]. The main objective is to develop a validated numerical simulation tool for describing the entrained flow gasification of biomass (cf. bioliq[®] process [5]). This paper presents work-in-progress and reports the recent experimental and numerical results for the entrained flow gasification of model fuels (ethylene glycol, 90 % ethylene glycol + 10 % wood-char) under atmospheric conditions. Three experimental campaigns have been carried out at the Research Entrained flow GASifier (REGA). Radial profiles of gas phase composition (CH_4 , CO , CO_2 , H_2) and temperature have been measured at burner distances of 300 mm and 680 mm. In parallel to the experimental campaigns, RANS based simulations have been performed using ANSYS Fluent. Turbulence-chemistry interaction has generally been described by the Eddy Dissipation Concept (EDC). EDC has been used in combination with two global reaction mechanisms for the entrained flow gasification of ethylene glycol: the HVII mechanism and the extended Jones-Lindstedt mechanism [3]. Devolatilisation and the heterogeneous reactions of wood-char with CO_2 and H_2O are computed using kinetics derived from measurements [6, 7]. The numerical results for the entrained flow gasification of ethylene glycol show good agreement with the measured data. In particular, the model based on EDC and the HVII mechanism predicts the gas composition well. Gas temperatures are slightly overpredicted. The numerical results for the gasification of slurry deviate from the experimental results concerning the gas phase composition. Further research needs to be carried out to close this gap.

1. Introduction

Entrained flow gasification (EFG) is one of the most promising gasification technologies and considers the conversion of low-rank fuels into high quality

syngas. To improve the knowledge of the gasification of biomass-based suspension fuels, the bioliq[®] process [5] has been realised at Karlsruhe Institute of Technology (KIT). Research on EFG was initiated in the frame of the Helmholtz Virtual Institute for Gasification Technology (HVIGasTech) [1-4]. The research is in particular based on a two-step approach: i) experiments and simulations at atmospheric conditions for improving and validating the sub-models used in the simulations; ii) experiments and simulations at high-pressure conditions for developing a numerical model for operation and scale-up of the entrained flow gasifier of the bioliq[®] process.

Experimental data from entrained flow-gasifiers is mainly available for the gas phase composition and temperature at the outlet of several gasifiers (see e.g. Chen et al. [8]). Radial profiles of gas phase composition and temperature were measured at the entrained flow gasifier of Brigham Young University (BYU), which was operated with coal at atmospheric conditions (see e.g. Brown et al. [9]).

Many studies on the mathematical modelling and simulation of EFG have been carried out in the last decades. Starting with one-dimensional models due to the limited computer resources at that time (see e.g. Wen [10]), CFD and RANS based models (see e.g. Marklund et al. [11]) are nowadays state of the art in the modelling of EFG in various geometries (e.g. two-stage up-flow, one-stage down-flow) and at various operating conditions. Such models are mainly based on two-equation turbulence models (e.g. standard $k-\varepsilon$, SST $k-\omega$) and global reaction mechanisms (Westbrook and Dryer [12], Jones and Lindstedt [13]) for the homogeneous kinetics. For the heterogeneous kinetics, the reactions of the fuel (generally coal) with CO_2 , H_2 , H_2O and O_2 are considered. Their reaction rates and the reaction rate of the devolatilisation process have usually been based on literature data or on measurements (see e.g. Brown et al. [9]). Radiation has often been calculated using discrete-ordinates method, P1 model or discrete transfer radiation model.

To the best of the authors' knowledge, no mathematical model is available which describes the EFG of biomass-based fuels and which has been validated using gas phase compositions and temperatures measured inside a gasifier. This paper provides an overview of the current status of the experiments at the atmospheric Research Entrained flow GASifier (REGA) and of the corresponding mathematical modelling.

2. Experiments

The REGA consists of a ceramic tube with an inner diameter of 280 mm and a length of 3000 mm. The heat loss of the system is minimized by electric heating of the reactor walls. The fuel (ethylene glycol or 90 % ethylene glycol + 10 % wood-char) is atomised using a twin-fluid external mixing atomiser and oxygen enriched air as gasification medium. A movable burner construction and flanges along the reactor axis allow measurements at a large continuous range of burner distances. Usually, radial profiles of gas phase composition and temperature are measured at

burner distances of 300 mm and 680 mm. The gas phase composition is determined as dry mole fractions of CH₄, CO, CO₂, H₂ and O₂ using standard gas analysers and a μ GC. Radial profiles of the gas phase temperatures are measured with type B double bead thermocouples with bead diameters of 300 μ m and 1500 μ m, which allow temperature correction by taking into account radiation. Further details concerning the test rig and the analytical equipment are given in Fleck et al. [2]. To improve the sub-models, several experimental gasification campaigns have been carried out under atmospheric operating conditions. In the first two campaigns, glycol was used as model fuel in order to exclude the impact of wood-char and to investigate the gasification at higher and lower adiabatic temperatures. For the third campaign, wood-char has been added and a similar adiabatic temperature has been selected as in the second campaign. Table 1 gives an overview of the experimental conditions.

Table 1. Experimental conditions of three gasification campaigns.

Campaign	Mass flow rate in kg/h			Adiabatic Temperature in K
	Fuel	O ₂	Air	
REGA-glycol-T1	12.56	7.11	9.04	2273
REGA-glycol-T2	12.42	6.54	3.76	1973
REGA-slurry1-T2	12.45	6.99	3.66	2041

3. Mathematical modelling

The numerical model is based on the software package ANSYS Fluent and a two-dimensional, axis-symmetric geometry of the REGA. Assuming a steady-state, the continuity equation, the momentum equations, the energy equation and a certain number of species equations have in particular been solved for the gas phase using a finite volume solver on an unstructured mesh. Additionally, equations according to the selected turbulence model and the selected radiation model have been solved. For describing turbulence, the standard k - ϵ model or the Reynolds stress equation model (RSM) has been applied by default while the SST k - ω model and the realizable k - ϵ model have also been tested. Consequently, the model is based on RANS (although all flow variables are Favre averaged). Radiation is taken into account by solving the radiative transfer equation by the discrete-ordinates method in $4 \times 8 \times 8 = 256$ directions. Due to the use of unstructured meshes, pixelation of 4×4 is also applied for reducing the control-angle overhang. The absorption coefficient is assumed to be constant. Its value of 0.53 m^{-1} has been calculated based on spectral line-by-line calculations using HITEMP-2010 and on a mean beam length. Detailed information about calculating the absorption coefficient and other material properties can be found in Mancini et al. [3].

The boundary conditions for the gas phase at inlet are defined by the mass flow rates given in Table 1 and temperatures measured near the atomiser (316 K; 317 K;

309 K). Additionally, the mass flow rates of purge nitrogen flow (0.64 kg/h; 0 kg/h; 0 kg/h) and the mass flow rates of infiltration air derived from balancing (1.93 kg/h; 0.59 kg/h; 0.69 kg/h) were considered. The boundary conditions at the wall are based on the no-slip condition, the linear law of the wall due to wall distances $y^+ < 5$ and an refractory temperature of 1200 °C in combination with a one-dimensional thermal resistance for the refractory with a depth of 50 mm.

The disperse phase is calculated using the Lagrange approach and the discrete phase model available in ANSYS Fluent and assuming an injection near the atomiser. The injection properties are based on measurements [2] and the total mass flow rate of the fuel given in Table 1. If glycol is used as fuel (REGA-glycol-T1, REGA-glycol-T2), the disperse phase at injection consists of liquid droplets containing ethylene glycol. If slurry is applied as fuel (REGA-slurry1-T2), the disperse phase at injection is modelled by a solid particle surrounded by a liquid layer. Material properties of liquid and solid phase are calculated using appropriate temperature dependent functions or proper constant values.

The reactions in the gas phase are described by the Eddy Dissipation Concept (EDC) in combination with a global reaction mechanism. Based on an extended version of the Jones-Lindstedt mechanism (eJL; see Mancini et al. [3]), the HVII mechanism has been developed consisting of six reactions [3]. These reactions describe the thermal decomposition of the evaporated fuel, the reaction with O₂ and reforming/gasification [3]. The reaction rates are based on comparisons with other reaction mechanisms (including the extended version of the Jones-Lindstedt mechanism and the GRI mechanism [14]). For the solid phase, the reaction rates for the devolatilisation and for the heterogeneous reactions with CO₂ and H₂O have been implemented based on the latest results of the collaborative research in the frame of HVIGasTech [6, 7].

4. Results

Figure 1 compares the impact of the global reaction mechanism on the temperature profiles and composition profiles at 300 mm and 680 mm. Obviously, both the HVII mechanism and the eJL mechanism reproduce the experimental data at 680 mm while the HVII mechanism predicts the experimental data at 300 mm better than the eJL mechanism. The temperature profiles are slightly overpredicted by both mechanisms.

Figure 2 shows the experimental and numerical results of the campaigns REGA-glycol-T2 and REGA-slurry1-T2. The numerical results have been computed using the HVII mechanism. For the gasification of glycol, the numerical results agree well with the experimental data. This is, however, only partially true for the gasification of slurry. The reasons for the deviations are still under investigation. To this end, experiments and simulations of one further campaign (70 % ethylene glycol + 30 % wood-char; REGA-slurry2-T2) are already on-going.

The numerical results were produced using RSM (REGA-glycol-T1) or standard $k-\varepsilon$ model (REGA-glycol-T2, REGA-slurry1-T2) due to lower computing time.

Sensitivity analysis has shown that the choice of the RANS turbulence model has only a small influence on temperature and composition.

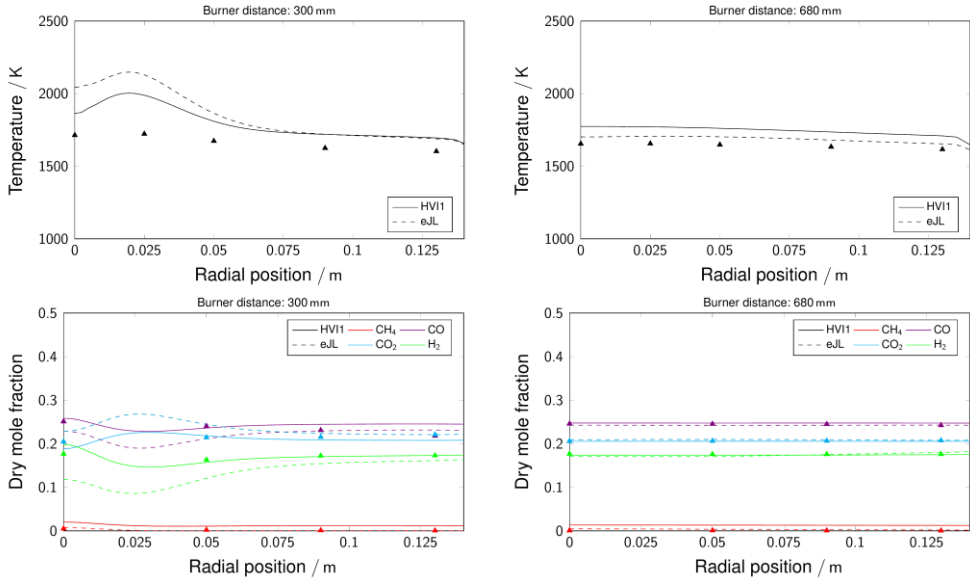


Figure 1. Comparison of experimental and numerical results of REGA-glycol-T1 campaign (as reported in Mancini et al. [3]).

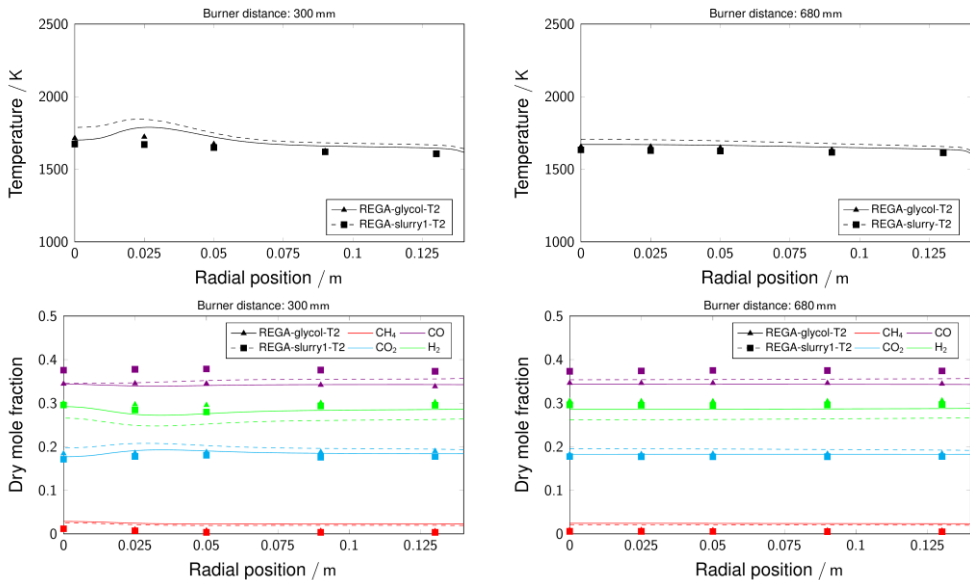


Figure 2. Comparison of experimental and numerical results of REGA-glycol-T2 campaign and REGA-slurry1-T2 campaign.

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