Elgázosító reaktor hidrodinamikai modellezése

Hydrodynamic Modelling of a Gasification Reactor

Gyurik Lívia[a], Egedy Attila[a], Jun Zou[b], Miskolczi Norbert[a], Ulbert Zsolt[a], Haiping Yang[b]

[a]*Pannon Egyetem 8200 Veszprém, Egyetem utca 10.*

[b]*Huazhong University of Science and Technology, Wuhan, 430074, China*

Összefoglaló

Tanulmányunkban egy két betáplálási és egy elvételi ponttal rendelkező elgázosító reaktor hidrodinamikai viselkedését vizsgáltuk tartózkodási idő eloszlás analízis segítségével. Megalkottuk a reaktor numerikus áramlástani (CFD) modelljét a reaktor impulzus és komponens mérlegegyenleteinek megoldásához. A tartózkodási idő eloszlás analízis céljából az áramlási egyenletek kiegészülnek egy komponensmérleggel. A szimulátorral történő megoldás hálófüggését a hibaráta számításával és a megoldáshoz szükséges idővel határoztuk meg. A tartózkodási idő eloszlás meghatározásához és a reaktoron belüli áramlási viszonyok jellemzéséhez impulzusszerű jelzőanyag betáplálást szimuláltunk. Egy jelzőanyagot tápláltunk a reaktorba 1 s-on keresztül egyidejűleg mindkét bemeneten 100 mol/m^3 koncentrációval, majd a jelölőanyag koncentráció adatait a reaktor kilépő felületén kiolvastuk a numerikus megoldásból. A CFD alkalmazásával történő vizsgálatok mellett egy cellás modellt is kidolgoztunk a reaktor áramlástani szerkezetének modellezésére, amit összevetettünk a CFD modellel kapott eredményekkel.

Summary

In our study the hydrodynamic behavior of a gasification reactor with two inlets and an outlet was numerically examined by the method of residence time distribution. We developed a Computational Fluid Dynamics (CFD) model of the reactor to solve the momentum and component balance equations of the system. The component balance equation was implemented to support the residence time distribution calculation. The mesh dependency of the CFD solution was checked by the error rate and calculation time. In order to characterize the mixing and flow within reactor pulse experiments were performed numerically. A tracer impulse was introduced for 1 s to both inlets at the same time with concentration 100 mol/m^3 approaching the Dirac delta function and tracer concentration at the outlet boundary of system was recorded. A compartment model in order to model the hydrodynamic structure of the reactor was also developed and compared to the results obtained by CFD model.

1. Introduction

Biomass gasification is an environment protecting technology as it consumes waste and turns them into energy or new valuable products. A gasification reactor burning biomass and producing energy modelled in this study [1]. There are several options to convert biomass into energy and fuels. The gasification reactor is usually constructed as fixed bed or fluidized bed reactor [2]. The production of biofuels by green technologies gives an alternative to fossil fuels aiming environment protection. Researches have already showed different ways of producing syngas from various components. As gasifying agents air, oxygen, steam or carbon dioxide can be used, all having different advantages [3]. There are two major groups of biomass, virgin and waste. They can be divided into subclasses i.e. terrestrial biomass, aquatic biomass as virgin biomass, municipal waste, agricultural solid waste, forestry residues and industrial wastes as waste biomass. Feedstock material can be wood, straw, sawdust, rice husk, algae, water plant, leaves, black liquor, waste oil and so on [4]. In our system cellulose was used as primary model component [5], and a laboratory scale reactor was constructed.

Computational Fluid Dynamics (CFD) is a widely used tool for modelling various systems. Using CFD we can effectively model and simulate the hydrodynamic behavior of systems by help of computers. Computer simulation allows analyzing and optimizing the behavior of real system without influencing it physically any way. Compartment models can be used to describe the hydrodynamic structure of complex systems using a set of elements of ideal reactor models, mixers and distributors. In our work we suggest a compartment model to model

the gasification reactor by applying a sequence of plug-flow reactors, continuous stirred-tank reactors, mixers and distributors. Kong et al. also researched the use of compartment models in case of gasification reactors [6]. While they built a detailed, complicated model, we defined a simpler model which was compared with our CFD model. We used MATLAB software for data processing and compartmental modelling, furthermore COMSOL Multiphysics software was used for CFD modelling.

2. Modelling approach

CFD methods use differential equations to describe and solve a time-spatial problem for a given geometry. In our case a gasification reactor with two inlets and one outlet was defined (Figure 1.a). The flow field was calculated with a laminar flow model using the momentum equation (Eq 1) and the continuity equation (Eq 2).

$$\rho(\mathbf{u} \cdot \nabla)\mathbf{u} = \nabla \cdot [-p\mathbf{l} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^{T})] + \mathbf{F} \quad (1)$$

$$\rho\nabla \cdot (\mathbf{u}) = 0 \quad (2)$$

The volume flow of steam and nitrogen were defined as boundary conditions at the inlet and outlet. The outlet was defined as a pressure boundary. All the other boundaries were treated as no momentum flux walls. Firs a stationary solution was calculated, the convective part of the component balance equation was calculated using the velocity field (Figure 1.b) obtained by solving the momentum balance equation.

In the further study we characterized the hydrodynamic behavior of reactor using residence time distribution analysis. For this reason we completed the Navier-Stokes equation with a component model (Eq 3). Simulating a tracer pulse experiment we introduced a tracer impulse for 1 s to both inlets at the same time with concentration 100 mol/m^3 and solved the component balance equation transiently. In general form of component balance equation the source term R was set to 0 in this simulation, but in the future researches the source term can be replaced by the chemical reaction or other sources. The wall boundaries are defined as no component flux boundaries.

$$\nabla \cdot (-D_i\nabla c_i) + \mathbf{u} \cdot \nabla c_i = R_i \quad (3)$$

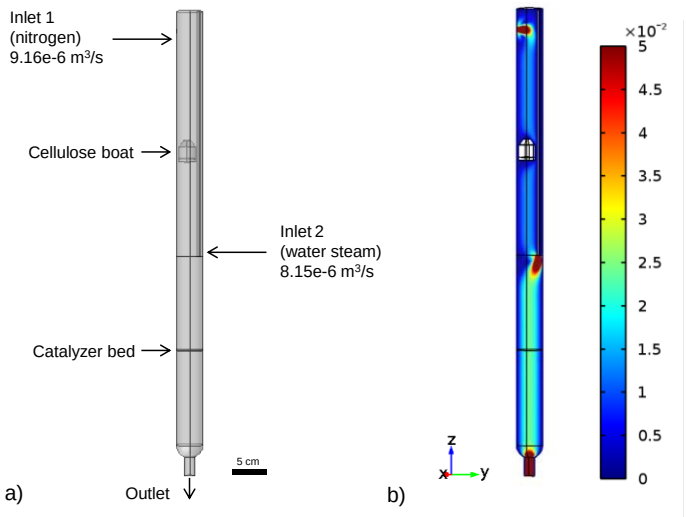

Figure 1. a) Inlets and flow rates of the gasification reactor. b) Velocity field contours of gasification reactor [m/s].

3. Results and discussion

Mesh independence study

In the mesh independence study we defined the 3D geometry of the reactor in the CFD software, and generated a calculation mesh with different qualities. In the case of mass balance increasing number of elements caused decreasing error rate but also increasing running time (Figure 2.a). Predefined meshes with 11.9 mm, 7.74 mm and 5.96 mm maximum element size were applied. Application of finer meshes resulted a relatively long computational time on a computer with 4 core 2.67 GHz processor and 16 GB RAM.

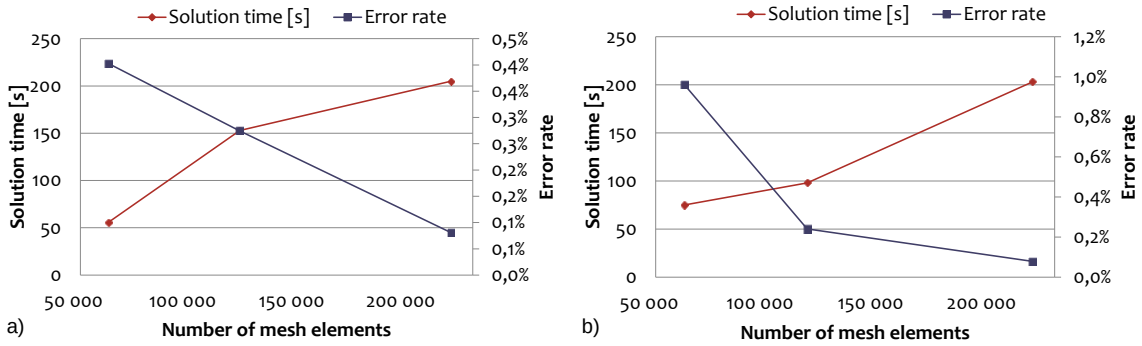

Figure 2. Effect of number of mesh elements on solution time and error rate in case of a) mass balance and b) component balance.

In the case of component balance similar correlation can be seen as Figure 2.b shows. Error rate is calculated as the absolute value of the difference between the inlet and outlet component mass divided by the inlet mass in percent. The mesh independence study shows that applying higher mesh quality increases the computational time. We selected the finest mesh of the examined three meshes, because this gives the best result in accuracy with reasonable solution time.

Residence time distribution analysis

Using the previously calculated velocity field of calculation domain we performed a pulse experiment by changing the inlet concentration in time to both inlets approaching a Dirac delta function. The tracer injection was applied as a rectangle function with 100 mol/m^3 for 1 s long duration. Figure 3 shows the residence time distribution function of the system detected at the outlet boundary. The red line is the component originated from the upper outlet (inlet 1, nitrogen), while the green curve represent the component originated from the lower inlet (inlet 2, water steam). Time delay in case of inlet 1 is longer since its origin located further from the outlet. Water steam reaches the outlet earlier as it is shown by the narrow peak section of the residence time distribution.

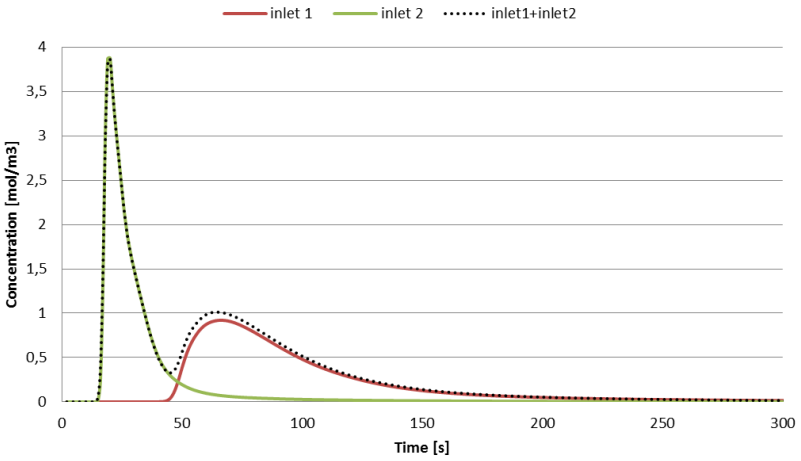

Figure 3. Residence time distribution of the system.

Compartment model

A system could be described by a sequence of compartments as plug flow reactor (PFR), continuous perfectly mixed reactor (PMR), mixer (M) or distributor (D) [7]. Developing a compartment model of reactor it was supposed that mixers and distributors have no volumes. Distributors have only one parameter to define, the percentages of inlets as its shown by equations (Eq 4–5) [8]:

$$F_{out,1} = \alpha F_{in} \tag{4}$$

$$F_{out,2} = (1 - \alpha)\, F_{in} \tag{5}$$

Following the structure of the real gasification reactor we constructed a compartment model shown in Figure 4. The proportion of compartments volumes applied in calculations was determined in two ways. First, the proportion of compartments volumes in the compartment model used in calculations (50%, 25%, 0.32%, 24.68%) were chosen correspondingly to the volume of the four main real reactor section (Figure 1a).

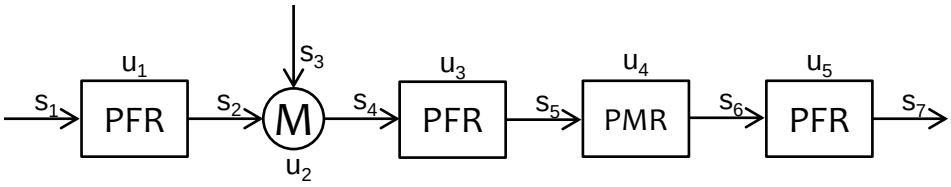

Figure 4. Compartment model of the reactor consisting of unites u_1–u_5 and streams s_1–s_7.

Figure 5a shows the comparison of residence time distribution obtained by CFD model and compartment model. We calculated an absolute and a squared error to characterize the difference between the results by the two models. In the case of compartment model the ideal plug flow reactors are approximated by a cascade of continuous perfectly mixed reactor. The time step of calculation was set to 0.2 s. The number of cascades in the calculation of plug flow reactor was set to 4 because we get the lowest absolute and squared error in this case. In the second case the proportion of compartments volumes was determined by application of an optimization tool (Particle Swarm Optimization [9], MATLAB) which resulted even less error (Figure 5.b).

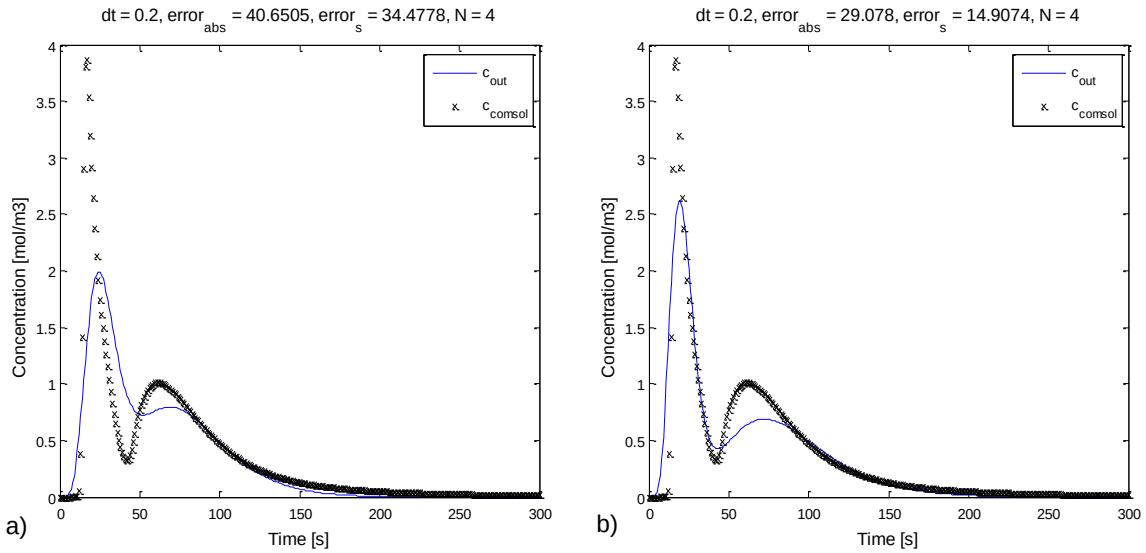

Figure 5. Residence time distributions of CFD and compartment model. a) volume of compartments are determined from the reactor structure; b) volume of compartments are obtained by using optimization algorithm.

The parameters and results are summarized in Table 1. The main difference can be seen in the case of first plug flow reactor, where the optimized algorithm provided a higher proportion of reactor volume at the first half of the reactor and the volume proportion of catalyst bed (unit 4) in which case the optimization tool gives a much higher proportion of compartments volume.

Table 1. Compartment model parameters and simulation results.

	real volume ratio of compartments	**optimized volume ratio of compartments**
cascade number in PFR model (N)	4	4
time step	0.2 s	0.2 s
absolute error	40.6505	29.078
squared error	34.4778	14.9074
Volume proportion of u_1	50%	60.08%
Volume proportion of u_3	25%	17.74%
Volume proportion of u_4	0.32%	4.44%
Volume proportion of u_5	24.68%	17.74%

4. Conclusion

A gasification reactor was examined in hydrodynamic point of view. The momentum and component balances of the reactor with prescribed geometry and operation parameters were solved by a CFD tool. The residence time distribution analysis was performed to characterize the hydrodynamic of reactor based on results calculated by CFD model. In addition to CFD modelling we approximated the system with a compartment model built up from ideal reactor models, mixers and distributors. The proportion of compartments volumes was determined in two ways: first using the real reactor structure, secondly an optimization tool was used to select

the optimal volumes of the compartments. In both cases the residence time distribution was calculated. The optimized compartment model shows a better agreement with the residence time distribution calculated by CFD model. Further development in the applied models research is planned by implementing chemical reaction kinetics into the component balance equation.

Acknowledgments

Authors thank to the National Office for Research and Innovation, within the framework of support for Hungarian-Indian (KTIA-DST) R&D&I co-operation program (TÉT_13_DST-1-2014-0003). This project has also received funding from the European Union's Horizon 2020 research and innovation program under the Marie Sklodowski-Curie grant agreement No. 643322 (FLEXI-PYROCAT).

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