# SIMULATION OF BIOMASS PARTIAL OXIDATION

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Abstract: Gasification of biomass by partial oxidation produces both syn-gas with high hydrogen content and explore energy of renewable sources. The objective of this work was to develop computer models of pilot reactor unit operated partial oxidation of rape meal/mineral oil suspension. The models were developed in process simulator ASPEN Plus based both on Gibbs free energy minimization and reaction kinetic approach. Alternative biomass characterizations were used: analogy with coal composition and representative compounds of biopolymer structure. Flow characteristic of gasification reactor was tested by CFD method in COMSOL Multiphysic. Simulated results were compared with pilot plant experiments with successful agreement.



## 1 INTRODUCTION

Nowadays hydrogen demand caused by deep fuel refining and the other sustainable processes leads to utilization of new raw materials. Simultaneously, extensive biodiesel production creates great amount of biomass wastes transcendent over feeding potential of farm animals. One of potentially useful process of hydrogen production from renewable natural sources seems to be partial oxidation (POX) and gasification of biomass material like rape meal from rape oil production and/or distillery slop originated from bioethanol (Tukač, 2009).

The goal of this work was to develop simulation models of pilot POX reactor working with mixture of fuel oil and biomass.

## 2 EXPERIMENTAL

Experimental pilot plant unit was constructed in UNIPETROL RPA Litvinov, consisted of water steam generator, continuous suspension batcher, gasification reactor equipped by co-annular feeding jet burner and water quench and tubular heat exchanger. Pilot POX reactor of I.D. 0.3 m and overall length 2 m was equipped by 5 x 3 kW electrical heating to reach temperature about 1200 °C. Suspension of dry biomass in mineral oil was partially combusted in oxygen - water steam atmosphere to produce carbon monoxide, dioxide and hydrogen contained gaseous product.

## 3 PROCESS SIMULATION

Two different approaches were used to develop mathematical models. First method consists in formulation of steady state balancing models created in process simulator Aspen Plus. Pseudo homogeneous CSTR reactor model was used to fit both reaction kinetics and chemical equilibrium on experimental data. Chemical and phase equilibrium was calculated by minimization of Gibbs function, Peng-Robinson equation of state with Boston-Mathias alpha function was used to describe real behavior of gases. Another modelling employs CFD capability of COMSOL Multiphysics (PDE solver by finite element method) to find steady state gas velocity, profiles inside of gasification reactor.

Complicated chemical composition was solved by concept of representative chemical compounds resulting in the same elemental composition as the original raw material.



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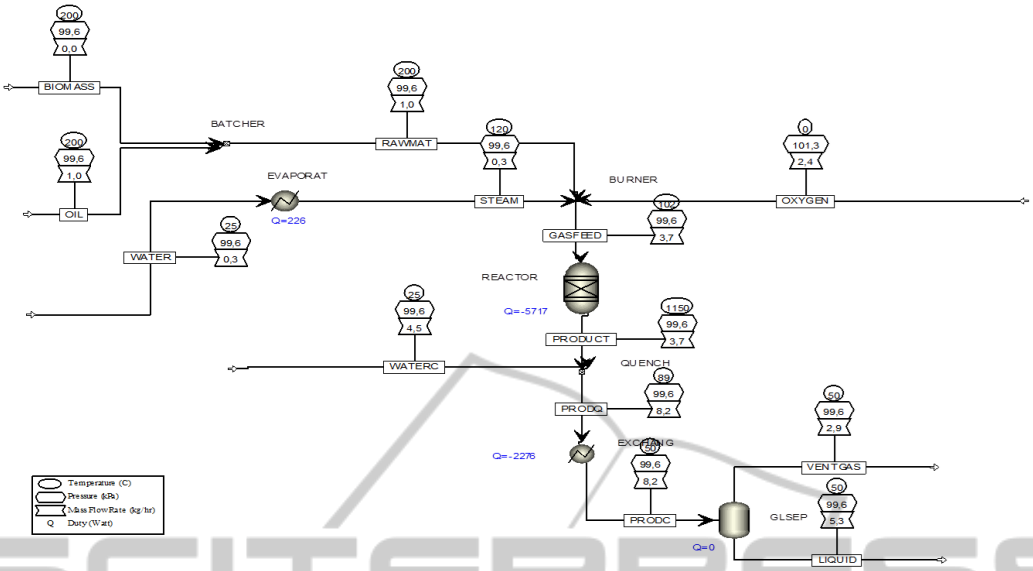


Figure 1: Aspen Plus flowchart of basic part of pilot POX unit.

In the Fig. 1 simplified flowchart of main part of pilot POX unit formulated in Aspen Plus is presented. Simulation model incorporates biomass, oil, water and oxygen input streams included water quench of flue gas after reactor.

Models of apparatus incorporate heat exchangers and phase separator. Two reaction models were used: i) chemical and phase equilibrium calculated by minimization of Gibbs function and ii) power law formal kinetics for gasification.

In the following Tab. I simulated results of chemical equilibrium for 10 % content of biomass in mineral oil are presented. Adiabatic temperature rise exceeds 800 K for both biomass tested, also prospected products concentration is very promising.

Table 1: Simulated results of gasification of biomass in oil suspension.

| Variable | 10 % rape meal | 10 % distillery slop |
|---|---|---|
| Adiabatic temperature in reactor, °C | 1038 | 1067 |
| Hydrogen portion in flue gases, % vol. | 48.7 | 48.5 |
| Carbon monoxide portion in flue gases, % vol | 35.8 | 36.0 |
| Molar ratio of carbon monoxide/dioxide | 8.08 | 8.44 |

Comparison of equilibrium simulation with experiments with 5 % wt. biomass-oil suspension gasification is shown in Fig. 2. Almost the same hydrogen concentration verifies results of simulation balance. On the other hand, lower experimental concentration of carbon monoxide together with higher value of carbon dioxide concentration implies that presumptions of both ideal mixing in reactor and/or complete chemical equilibrium are not fulfilled. Also method to fit apparent equilibrium temperature (Bruggemann, 2010) corresponding to experimental composition was treated. The resulting temperature approach was found cca -500 °C and both carbon oxide and methane concentration are affected. In this case, it is possible to see in the Fig. 2. better agreement of that simulation with experimental results.

Fitting of experiments by simple power law kinetic of partial oxidation, water gas shift, steam reforming and carbon monoxide oxidation the good agreement was found with published data (Robinson, 2008).

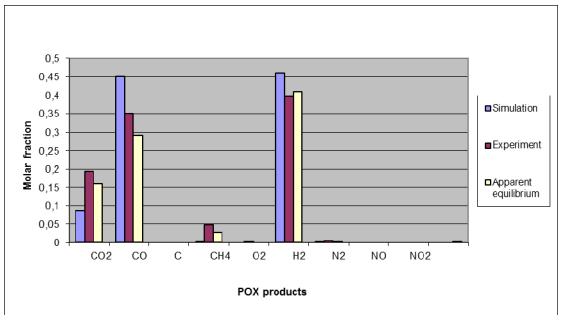


Figure 2: Examples of 5 %wt. biomass in oil gasification by oxygen – water atmosphere, mean experimental temperature 1152 °C, apparent equilibrium temperature 672 °C.

Hydrogen production depend both on oxygen and water steam ratio to biomass and hydrocarbon raw material mixture and also on flow characteristic and internal mixing in the reactor. Distribution of residence time of biomass particles in the reactor affects results due to different rate of consecutive reaction steps: pyrolysis, water gas shift and steam reforming reactions. CFD modelling can help to understand complex phenomena in the reactor. To evaluate axial mixing in the reactor axial symmetric cylindrical model in COMSOL multiphysics was created. Fluid flow was described by Navier Stokes equation and turbulence by k-ε model (Cammarata, 2007). Resulting flow character is presented in Fig. 3, exhibiting vortexes in upper and bottom reactor part and main stream in reactor axis. To choose appropriate hydrodynamic model (Bruggemann, 2010) some RTD measurement should be necessary.

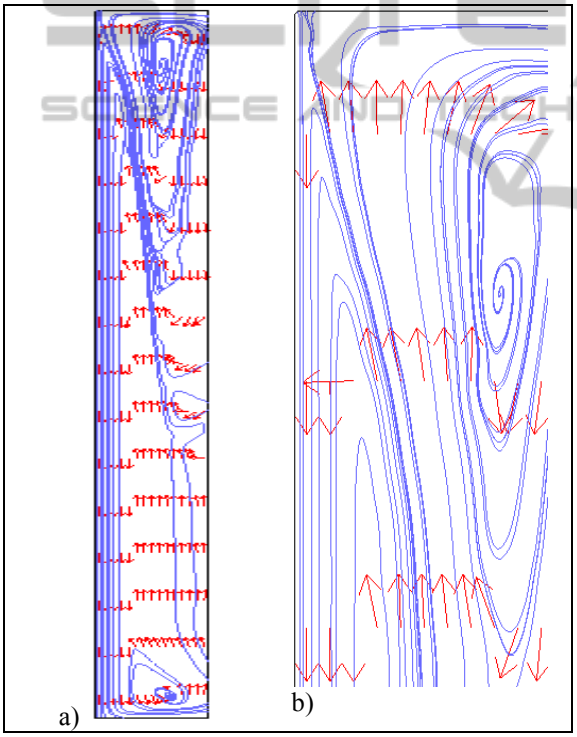


Figure 3: a) Velocity stream lines in longitudinal cross-section of axial symmetric reactor model. Left edge – axis, right border – wall.. b) Detail of jet nozzle vicinity.

## 4 CONCLUSIONS

Variant thermodynamic calculations of equilibrium balances of biomass partial oxidation were made by process simulator Aspen Plus. Prospective results were found both for rape meal and distillery slops oil suspension oxidation.

Comparison of equilibrium reactor model with preliminary experiments shows good agreement, but for existing deviations mixing structure in reactor is suspected. The best results were acquired by model with equilibrium temperature approach.

CFD results of 2D axial symmetric FEM model invoke a need for experimental RTD identification of axial mixing flow character.

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