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Subject: Short Term Scientific Mission
Reference: COST Action CM1404
Host institution: Norwegian University of Science and Technology (NTNU), Faculty of Engineering, Department of Energy and Process Engineering
Host Supervisor: Prof Dr Terese Løvås
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1. Purpose of the STSM

The aim of this Short-term Scientific Mission (STSM) was to establish contact with the NTNU, Faculty of Engineering, Department of Energy and Process Engineering, as well as to obtain new references on past and present research needed to further develop the theoretical and conceptual tools used in my current research work (modelling thermochemical processes).
Furthermore, as I am doing research in biomass and waste pyrolysis and gasification process (experimental and modeling approach) at home University (UBFME), visiting NTNU provided me with the opportunity to network with NTNU research team, under supervisor of prof Dr Terese Løvås, as well as expose, compare, and evaluate my work in relation to current relevant work being undertaken on the same research field.
At the beginning the plan was to collaborate on particle modelling and fuel NOx kinetic.
Considering that visit was too short to get deeper insight into the principle of modelling work and relevant computational infrastructure, the plan of activities was, in site, changed.
Considering that, on one hand my current research interest are modelling of pyrolysis, gasification and combustion modelling (analysis of different operating parameters on product yields), and on other hand one of research activities of NTNU research team (Kathrin Weber) is stochastic reactor modeling of biomass pyrolysis and gasification, research focus was directed to the analysis of the results from my research and research of college Kathrin Weber.
Generally, the purpose of the STSM:
1. Analysis of two modelling approach for biomass pyrolysis and gasification process, analysis of the results of the research.

2. Presenting research activities of (NTNU, SINTEF and UBFME) in order to establish possible collaboration research work inside the SmartCats Cost Action.

2. Description of the work carried out during the STSM

a) Theoretical contextualisation of the international and European research
Updating the theoretical framework of the research task, collecting newest results from NTNU research team which are published in sci journals
b) Research contextualisation in the host (NTNU) research team
The NTNU research team, Kathrin Weber, developed a partially stirred stochastic reactor model for the modeling of biomass pyrolysis and gasification process. Kathrin gave me an opportunity to extend my research about pyrolysis and gasification process modelling, by exchanging experience, knowledge and by sharing methodologies and results. In particular, I was able to learn about the analysis and explanations they found in their researches in order to improve my interpretation of the results. The discussion and comparison was undertaken considering theoretical and experimental aspects relating to biomass pyrolysis and gasification process.

3. Description of the main results obtained: writing task

The deterministic model

The model that I`m currently developing is a zero-dimensional mathematical model for downdraft gasification of biomass. This model involves main gasification sub-processes (drying, pyrolysis, gasification) and their products (Figure 1).

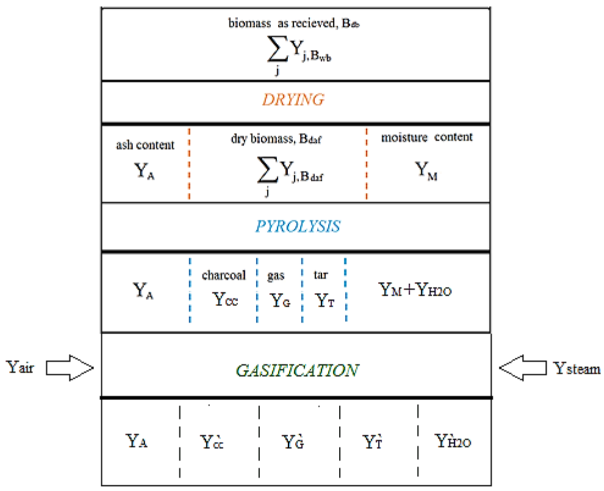

Figure 1 Overall mass balance to the biomass gasification process. The presented quantities (Y) are mass ratios referred to the dry ash-free part of biomass

The model consists of energy, mass and elemental balance equations and empirical relationships between the product yield and pyrolysis temperature. The three most common gas–solid reactions that occur in the gasification zone considered in modeling are: the water–gas or steam reaction, the Boudouard reaction and the methanation reaction. The equilibrium constants for each reactions are empirical and taken from literature. The proposed model successfully predicts behaviours of different types of biomass during a gasification process (yield and composition of products) and is a useful tool to simulate the influence of different operating parameters (equivalence ratio, air preheating, steam injection, and oxygen enrichment) on gas characteristics.

The stochastic model

The model, that is currently developed and is further developing, at the NTNU research team, is partially stirred stochastic reactor model for the modeling of biomass pyrolysis and gasification. In this zero dimensional stochastic reactor model, the state variables, which are heterogeneously distributed in the reactor, are described and modelled with probability density functions. Also, a relatively simple chemical mechanism was coupled with the stochastic reactor model. This model is made suitable for biomass pyrolysis and/or gasification through proper treatment of the gas-solid phase interaction for biomass conversion through drying, devolatilization, char reactions and gas phase reactions. This proposed model successfully predicts behaviours of different types of biomass during a gasification process (yield and composition of products) and is a useful tool to simulate the influence of different operating parameters (equivalence ratio, air preheating, steam injection, and oxygen enrichment) on gas characteristics.

Models comparison

The input parameters:

1. Beech wood composition:

Table 1 Proximate and Elemental Analysis of beech wood (as received) [1]

Proximate Analysis	
Moisture	9.04 wt%
Ash	0.61 wt%
Volatile matter	76.70 wt%
Elemental Analysis	
C	45.05 wt%
H	5.76 wt%
O	39.41 wt%

2. Temperature of reactor: 1300, 1400, 1500, 1600 and 1700^{o}C

The deterministic model was compared with stochastic model [1] and Qui et al. [2] experimental results. The compared results are presented in Figure 1. It should be notedd that yield of CH_4, in deterministic model, was taken from experimental results.

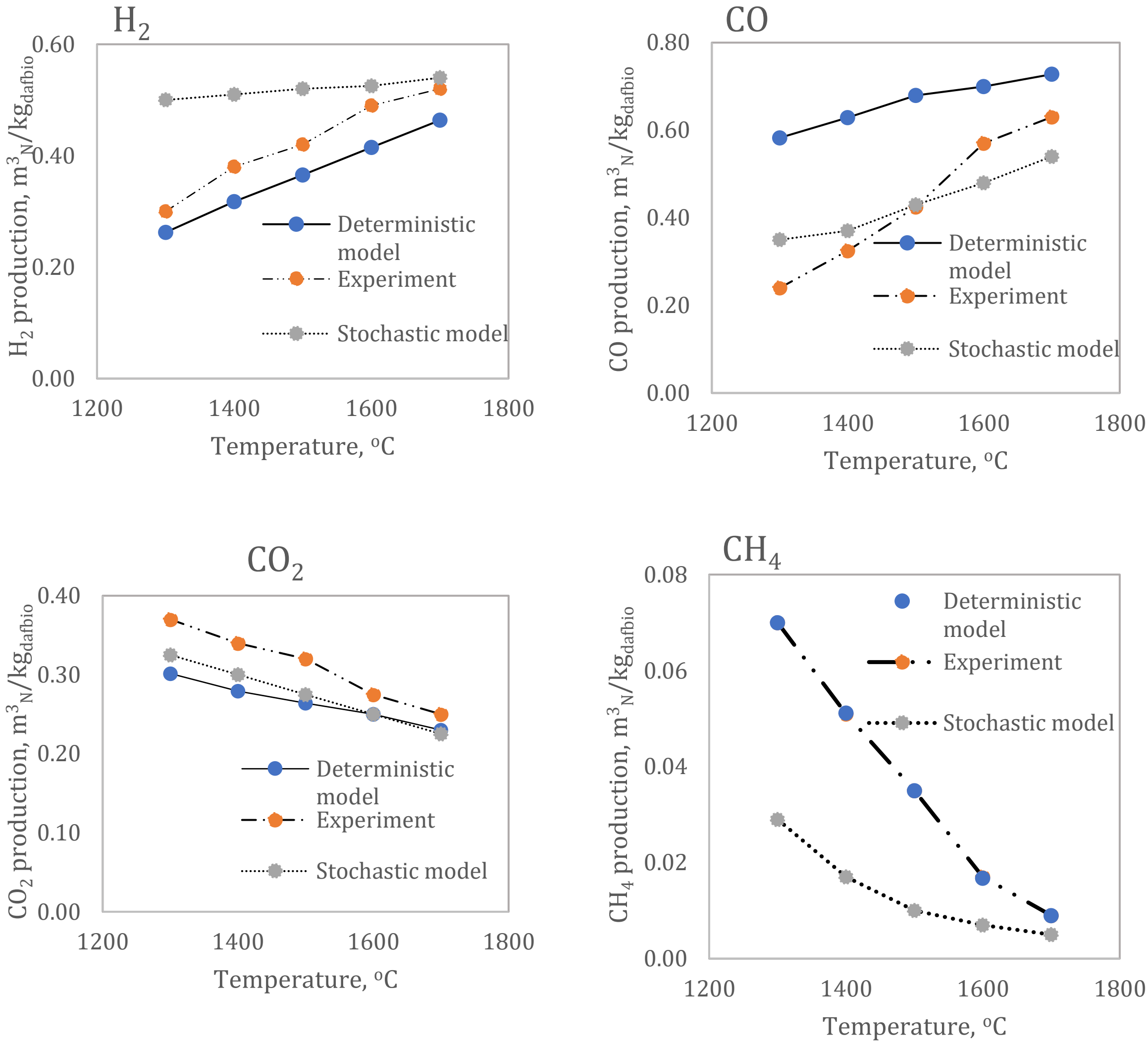

Figure 1. Comparison of predicted results from the deterministic and stochastic model with experimental results

The deterministic model captures the overall effect of temperature on all the product gases well. Hydrogen production is underpredicted by deterministic model, and over-predicted by the stochastic model. Carbon monoxide is overpredicted by deterministic model. For stochastic model, at the reactor temperature above 1500 °C, CO is slightly overpredicted, and for temperatures above 1500 °C CO is underpredicted. Carbon dioxide is in good agreement with experimental data. The lowest reactor temperature gives the largest deviation from the experimental measurement. At the highest temperature, the model performs better.

Both models (deterministic and stochastic), captures the overall effect of temperature on all the product gases well. However, the differences in gas yield trends should be clearly analysed and explained. The next step in research, is implementation of stochastic rector model approach in order to understand, analyses differences in modelling results (e.g. importance of kinetic mechanism).

4. How the STSM has contributed to the Action's aim

"SMARTCATS COST Action aims to set-up a Europe-wide network of leading academic and research institutions and key industries to promote the use of smart energy carriers on a large scale in order to increase fuel flexibility and carbon efficiency of energy production and to support distributed energy generation strategies", (http://www.smartcats.eu). Regard to mention, this STSM gave opportunity for network establishing between UBFME and NTNU. The plan for further collaboration work was made (experimental and modelling work exchange in field biomass and waste to energy).

4. Future collaboration with host institution (if applicable)

This mission has passed in good spirits and understanding. In the future, I will stay in contact with prof Dr Terese Løvås and her research team to follow up on the experimental and modeling results in field of biomass and waste pyrolysis and gasification, but also to keep them updated about my own experimental and modeling results. Further collaboration would be beneficial hopefully for both sides.

5. Foreseen publications/articles resulting or to result from the STSM (if applicable)
Publications resulting from STSM activities must acknowledge COST Action CM1404

If further analysis of two modelling approach (deterministic and stochastic models) gives valuable results, hopefully results of this analysis would be published .

6. Confirmation by the host institution of the successful execution of the STSM (attached the original document)

Kindly ask You, please see the pdf document written by the host, prof Dr Terese Løvås, attached to the email.

7. Publications resulting from STSM activities must acknowledge COST Action CM1404

YES

Financial Report

Flight Costs	561 EUR
Accommodation	335 EUR
Subsistence	250 EUR
TOTAL	**1146**

I would like to express my special gratitude and appreciation to the MC Chair of COST Action CM1404 (SMARTCATS), Dr Mara de Joannon, for her support and guidance during my STSM. Furthermore, I would like to record my appreciation to the MC of Cost Action CM1404 (SMARTCATS) for granting the funding to allow me to carry out this STSM.

I would like to thank prof Dr Terese Løvås, Kathrin Weber and other members of the NTNU research team for friendly hospitality and given support.

References

1. Weber, K., et al., *Stochastic reactor modeling of biomass pyrolysis and gasification.* Journal of Analytical and Applied Pyrolysis, 2017. **124**: p. 592-601.
2. Qin, K., et al., *Biomass Gasification Behavior in an Entrained Flow Reactor: Gas Product Distribution and Soot Formation.* Energy & Fuels, 2012. **26**(9): p. 5992-6002.