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Activation energy prediction of biomass wastes based on different neural network topologies

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ABSTRACT

The present paper discusses the thermal data prediction performance of ANN for more than one biomass as well as the reliability of this ANN predicted data in the further steps. Lignocellulosic forest residue (LFR) and olive oil residue (OOR) were selected as biomass feedstocks. The thermal data prediction performance of ANN was performed based on two approaches by developing; *i)* two individual networks for each feedstock, and *ii)* one-network for both feedstocks. After fixing the main structure of the networks, optimization studies were carried out to determine the best network configuration. In this way, it was also aimed to discuss the effect of internal ANN parameters to the overall prediction capability for more complex problems. At the final step, the predicted data was applied to calculate the activation energies based on three conventional kinetic models and the results were compared with the ones calculated using experimental thermal data. In the end, it was concluded the experimental thermal data fitted quite well to the ANN predicted data ($R^2 > 0.99$) but more complex network topology was required for combined network due to the complexity of the dataset. Most importantly, it is shown that the predicted data can be applicable for the further steps such as in the calculation of the activation energies using different models.

1. Introduction

The increasing concerns in the use of fossil sources such as security problems, sudden price changes in the market as well as their negative impact on the environment have been forcing countries to increase the share of alternative sources in the energy production. Biomass stands as a near-term renewable and alternative energy source, since it can be considered as CO_2 neutral due to its much less contribution to the increase of the greenhouse gases unlike fossil fuels [1,2]. Additionally, it is possible from biomass to produce not only energy but also other value-added chemicals by applying different technologies [3,4]. Pyrolysis is the thermal decomposition of biomass to produce solid, liquid and gas products in the absence of oxygen. One of the main reasons which makes pyrolysis attractive is the flexibility of the process that allows to produce variety of products and chemicals depending on the operational conditions. Moreover, compared to other thermal methods such as gasification and combustion, pyrolysis is known as the common step of thermal processes which enables a detailed characterization of thermal and kinetic behaviors that can be helpful for the further steps of the operation. Investigations into pyrolytic behaviors of biomass at high temperature region play an important role in terms of gaining insight about the process, providing a better understanding in the process parameters as well as designing the equipment.

Thermogravimetric analysis (TGA) has become an ordinary and necessary laboratory procedure to analyze thermal behaviors of different materials [5–7]. TGA provides information on the continuous mass loss characteristics of the samples to clarify their behaviors [8,9]. Nowadays, most of the researchers are attempting to apply computational methods for the prediction of thermal data to reduce the number of the ordinary laboratory procedures. Artificial Neural Network (ANN) has a comprehensive ability to establish a relationship between input-output data due to its approximating ability for arbitrary non-linear data sets [10,11]. Therefore, ANNs can also be applied to model biomass decomposition considering the complexity of the thermal data belong biomass decomposition. In the literature, it is possible to find variety of studies in which ANN is applied as an alternative modelling tool, depending on the type of the thermal process such as pyrolysis [12], gasification [13,14] and combustion [15].

In our previous study, we developed an ANN model that can predict the thermal behaviors of refuse derived fuel (RDF) by discussing the effects of network parameters such as number of the hidden layer(s), number of neurons in the hidden layers, and the type of the transfer

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Nomenclature

A	pre-exponential factor (min^{-1})
α	conversion
β	heating rate ($K\,min^{-1}$)
E	activation energy (kJ/mol)
$f(\alpha)$	function expressing dependence of the reaction rate on the conversion
k	reaction rate constant
n	order of the reaction
R	universal gas constant ($8.3145\,J\,mol^{-1}\,K^{-1}$)
R	regression
t	time (min)
T	temperature (K)
T_m	temperature at maximum reaction rate (K)

Abbreviations

ANN	Artificial Neural Network
BP	Back Propagation
DTG	Derivative Thermogravimetry
FWO	Flylnn-Wall-Ozawa Method
KAS	Kissinger-Akahira-Sunose Method
LFR	Lignocellulosic Forest Residue
LM	Levenberg-Marquardt
MSE	Mean Square Error
OOR	Olive Oil Residue
RDF	Refuse Derived Fuel
TGA	Thermogravimetric Analysis
logsig	Log-sigmoidal Nonlinear Function
purelin	Linear Transfer Function
tansig	Tan-sigmoidal Nonlinear Function

functions [16]. It was concluded that once the network is optimized carefully, it is possible to predict thermal behaviors of biomass accurately. However, in case of a new feedstock, all of these optimization steps should be repeated. In addition to these challenging and time consuming procedure, testing the applicability of ANN predicted thermal data in further steps (like activation energy calculation) stands as another crucial point. Therefore, in the present study, a deeper discussion was carried out by asking the question of *"If an ANN model was developed for more than one feedstock to predict the thermal behaviors, is the thermal data obtained from this network be applicable in further steps?"* To answer this question, ANN predicted thermal data was used to calculate pyrolytic activation energies based on different kinetic models and the results were compared with the ones calculated using experimental data. Using ANN predicted thermal data in the calculation of the activation energy instead of directly predicting the activation energy (setting activation energy as output of ANN) as in some of the studies in the literature [17,18] can be beneficial from many aspects. First of all, estimating thermal data allows flexibility to perform different types of

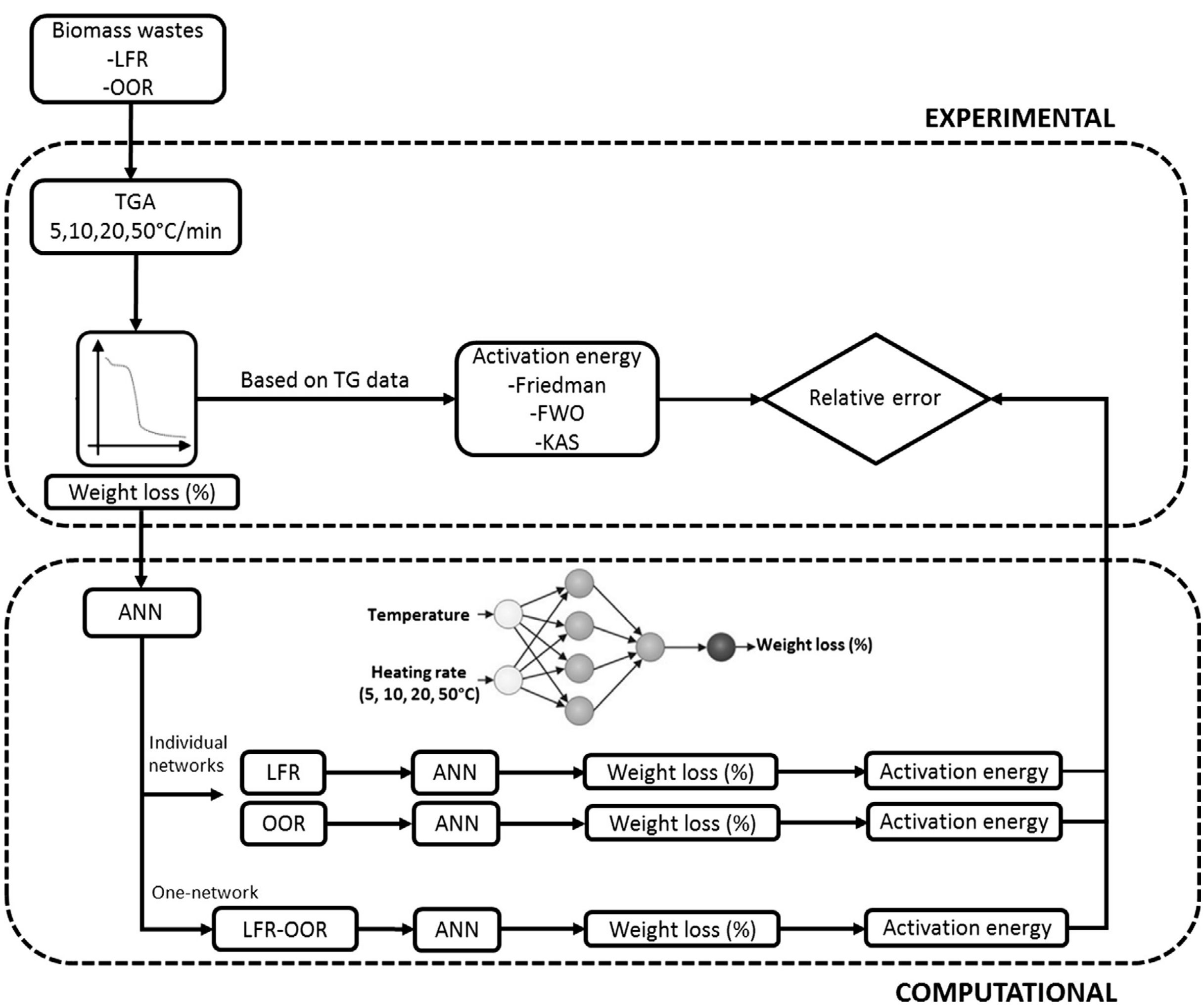

Fig. 1. The overview of the pathways followed in this study.