



## Research article

# Computational modelling of the condensation of fast pyrolysis vapours in a quenching column. Part B: Phase change dynamics and column size effects



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## ABSTRACT

The aim of the present work is to provide detailed information on the phase change dynamics of a discrete representation of the pyrolysis vapours in a direct contact heat exchanger (disc and donut quenching column). Eleven compounds were chosen to represent the most common chemical groups found in bio-oil (i.e. acids, aldehydes/ketones, pyrolytic lignin and water). The pyrolytic lignin group is represented through mono-phenolic compounds (i.e. phenol, coniferyl alcohol, guaiacol) whereas the effect of sugar and lignin derived oligomers is neglected. The work aims to identify how different numbers of disc and donut pairs (stages) 3, 5 and 9, affect the condensation performance of the column. The saturation vapour pressures of the individual compounds were calculated based on corresponding states correlations. It is shown that heavy compounds, such as guaiacol, phenol and coniferyl alcohol condense rapidly even with a low number of stages, whereas an increased number of stages is needed to completely capture the heavier acidic (butyric acid) fractions. In all cases, the majority of the acidic fraction (acetic acid and propionic acid) and water were only partially condensed, whereas formic acid and the aldehyde fraction (propanal and pentanal) were not condensed at any stage of the process.

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## 1. Introduction

The demand for fossil fuels has been increased over past few decades due to the rapid growth in terms of global industrialization and development. Moreover, the depletion of fossil fuel reserves coupled with the increasing energy consumption and greenhouse gas emissions poses a new set of challenges. These factors put thrust on the utilisation of renewable energy resources, such as biomass, solar and wind energy. In addition, many countries pledged to reduce the greenhouse gases further intensified the need for renewable energy sources [1].

The use of biomass as a source for energy is one of the alternatives that can contribute to decreasing the share of fossil fuels [2]. Moreover, this will also lead to the reduction of greenhouse gas emissions [3]. When compared with other renewable energy sources, biomass stands as the only source for solid, liquid and gaseous fuels. Biomass fast pyrolysis presents certain advantages among all the conversion techniques available for the generation of liquid fuels [4]. This process can provide a liquid fuel that has the potential fuel in any static heating or electricity generation application [5,6].

Fast pyrolysis vapours require to be rapidly condensed for optimum liquid bio-oil yields. The primary requirement for higher liquid bio-oil

yields is the rapid condensation of the condensable pyrolysis vapours [8–11]. Hence, high heat transfer rates, carefully controlled temperatures, the residence time of pyrolysis vapours in the reactor are the most significant factors that affect the process. The presence of non-condensable gases in the system poses significant heat and mass transfer resistance as well as low partial pressures that significantly limit the efficient collection of the liquid product. In the case of the conventional heat exchangers, an inherent problem of preferential deposit accumulation of lignin-derived components, which eventually leads to liquid fractionation, is also present [7]. These depositions typically cause blockages of the pipelines and consequently the heat exchanger itself. Moreover, due to the improved thermal performance of direct contact condensers, up to 60% less cooling medium is often required than that needed in indirect contact condensers [12]. Several types of direct contact condensers are deployed in fast pyrolysis liquid collection systems like spray columns and quenching columns. These direct contact heat exchangers, significantly minimise the previously stated limitations and provide greater contact area between the coolant and the vapours, which in turn aids the rapid cooling of the latter as well as the capturing of the condensed aerosols.

Recently, the sequential condensation of the pyrolysis vapours is gaining significant popularity [13–15]. The majority of the experimentalists [15–21] deployed series of indirect condensers to achieve sequential condensation whilst few others [22–24] used direct contact condensers. The advantage of sequential condensation is that different fractions of

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bio-oil with different compositions can be collected so that the partial upgrading process can be achieved within the pyrolysis process. This will also contribute to the overall thermal efficiency of the plant [25,26]. For this reason, it is essential to understand the physical behaviour of flows within the liquid collection system so that the efficient column designs can be developed.

According to Bridgwater [27], one of the most essential features of fast pyrolysis for the production of liquid fuels is the low vapour residence time. The vapour residence time refers to the time taken by the vapour from its generation in the reactor to the condensation in the liquid collection system. The optimum vapour residence time is typically 2 s, which minimises the undesirable secondary reactions that take place in the vapour phase. Secondary cracking tends to increase the percentage of non-condensable gases in the expense of the final liquid bio-oil [28,29]. This introduces a significant challenge in the design of efficiently operating quenching columns using empirical relations, which is restricted by the high complexity of the process. The gas–liquid interactions in terms of momentum, heat and mass transport, result in complex flow regimes that are difficult to be predicted by experimentation alone. The thermodynamic condensation model developed by Westerhof et al. [13], based on the well-known Rachford–Rice formulation [30], provided an insight on how the water yield can be controlled during the condensation of pyrolysis vapours. In the works of Tumbalam Gooty et al. [31,32], the results of the models developed in HYSYS tool were utilised as a guide to standardise the practical performance of the fractional condensation series. However, these models can only provide the overall balances and lacks the spatiotemporal details of the parameters within the condensing unit which are necessary to develop efficient designs. Under these considerations, the employment of computational methods to provide an insight on the physical phenomena present in the process (i.e. hydrodynamics, heat transfer and phase change phenomena) becomes increasingly necessary.

Various modelling studies have been undertaken in the modelling of the hydrodynamics of sieve tray columns [33–36]. So far, most of the modelling studies performed in the field of pyrolysis technologies are either focused on particle dynamics [37] or chemical conversion modelling [38] within the fluidised bed reactors. A comprehensive review on the mathematical modelling on pyrolysis reactors has been recently presented in the works of Sharma et al. [39]. Some researchers conducted computational fluid dynamics (CFD) analysis on reactor hydrodynamics and its thermochemical performance with a focus on reducing the residence time of vapours and achieving better separation efficiency [40,41]. However, only few research studies have been conducted in the numerical modelling of the condensation of pyrolysis vapours [42]. In this study, the condensation of the mixture of pyrolysis vapours, in the presence of non-condensable gases, is simulated in an indirect contact heat exchanger. The vapours are treated as ideal gases, whilst the vapour mixture is treated as a unique phase without distinct chemical species. In a later work [43], the assumptions imposing restrictions on selective condensation of different species was improved by treating the vapour phase as a mixture of distinct species. However, the authors have not identified a single study on the numerical modelling and simulation of the condensation of fast pyrolysis vapours within a quenching column.

The aim of the current study is to model the phase change phenomena due to condensation occurring within a quenching column. The gas–liquid interactions are simulated using the immiscible Eulerian – Eulerian approach. The assessment of the hydrodynamic performance of the quenching column has been presented in the first part of this study [44]. The chemical thermodynamics governing the condensation process have been incorporated in user-defined subroutines to suit to the flow regimes within the quenching column. The numerical model has been applied for the determination of the optimum number of stages within the quenching column and its effect on the condensation of individual species. The CFD results clearly show the impact of the

number of stages, temperature and pressure on the relative saturation of the individual species. Also, the effect of the species volatility on the phase change characteristics is thoroughly analysed and discussed.

## 2. Experimental conditions

Experimental investigations have been conducted at Aston University, based on the ablative pyrolysis process described by Peacocke et al. [45], for the production of liquid bio-oil. The pyrolysis reactor is designed to operate at a biomass feeding rate of 5 kg/h; however, due to feeder limitations the feeding rate was limited to 3 kg/h [46]. The liquid collection system of the pyrolysis rig comprised of a quenching column coupled with an electrostatic precipitator. The dimensions of the quenching column are based on the maximum intended gas flow rates from the pyrolysis reactor, as well as the flooding factors.

The original (baseline) design of the quenching column and the equipment has been designed for a total gas (i.e. gases plus pyrolysis vapours) flow rate 0.0044 m<sup>3</sup>/s at a temperature of 400 °C. The gaseous composition was estimated based on Toft's [47] empirical relationship. Thus, the total gas composition consists of 87% N<sub>2</sub> by volume, whilst the remaining 13% consists of condensable and non-condensable gases.

Octane at –5 °C and at a flow rate of 0.025 kg/s, has been used as the direct contact cooling medium because of its immiscibility with the highly oxygenated hydrocarbons present in the final liquid bio-oil product. The design specifications of the discs and donuts inside the quenching column are given in Table 1. The experimental findings reported flooding of the quenching column at the design gaseous flow rate of 0.0044 m<sup>3</sup>/s. However, the design modifications suggested in the first part of this study eliminated flooding phenomena are also highlighted in Table 1.

## 3. Condensation model

The condensation model used in this paper is an extension to the works of Papadakis et al. [42] and Palla et al. [43]. In the former work, the condensation model was presented using a uniform vapour composition, whereas in the latter one, the model was developed for the indirect contact condensation and modelled using species transport. The current model extended the scope to direct contact condensation with some limitations as described below. The pyrolysis vapour is represented with 11 species. Each individual species is treated as an individual compound which is condensed according to its saturation vapour pressure. The condensation model in this way enables the prediction of the pyrolysis vapour composition accurately at each stage, once the initial vapour composition is known. The inlet pyrolysis vapour composition is highly dependent on the type of feed used during the pyrolysis process and type of reactor and its conditions. These compositions further suggest the type of application for which the bio-oil produced [48]. The selection of the number of chemical species and their corresponding initial volume fractions can be modified depending on the chemical compounds of interest. A more comprehensive classification and grouping can be found in the works of Garcia-Perez et al. [49] where they developed a characterisation approach to determine the bio-oil composition in terms of macro-chemical families.

The pyrolysis vapours used in this analysis were represented in a discrete form by 11 chemical species typically found in bio-oil. The selected species are listed in Table 2, and have been taken from the bio-oil composition used in the work of Brett et al. [50]. This discrete composition is an equivalent representation of the continuous thermodynamics model used in the study of Hallett and Clark [51], which in turn is based on molecular weight distributions of specific chemical groups found in bio-oils (i.e. acids, aldehydes/ketones, pyrolytic lignin and water). It has to be pointed out that in the current work the effect of lignin and sugar derived oligomers has been neglected, whilst the pyrolytic lignin group is simplified to a mono-phenolic representation through phenol, guaiacol and coniferyl alcohol. Whilst making a discrete

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