HYDRODYNAMIC MODELING OF A DIRECT CONTACT HEAT EXCHANGER USED FOR BIO OIL CONDENSATION

Kiran Kumar P.V.S.^{1, 2}, K. PAPADIKIS¹ and Sai GU^{*1}

¹ Civil Engineering Department, Xi'an Jiao tong-Liverpool University, Suzhou, Jiangsu Province, CHINA. ² School of Engineering, University of Liverpool, Liverpool, U.K. *Corresponding author, E-mail address: Sai.Gu@xjtlu.edu.cn

ABSTRACT

Quenching columns are used for condensing pyrolysis vapours to produce liquid bio-oil using the direct contact heat exchange method. The fluid flow inside this type of equipment is quite complex involving the interaction between multiple phases. In the current paper, the hydrodynamic behaviour of a quenching column utilised in ablative fast pyrolysis experiment is modelled. Liquid octane is circulated inside the condenser as a cooling medium. Pyrolysis gaseous components were modeled by non-condensable gas nitrogen. This gas is introduced at the bottom of the column where it comes in direct contact with the cooling liquid. The Eulerian - Eulerian model with immiscible option is used to analyse the gas liquid interactions. The CFD predictions validated the flooding phenomena occurred in the quenching column during the experiments. Design modifications are also discussed together with the implications of those on the final performance.

NOMENCLATURE

A_{c}	Curtain area	m^2
$A_{\rm w}$	Window area	m^2
d	Droplet/ bubble diameter	m
g	Gravitational acceleration vector	m/s ²
h	Specific enthalpy of the phase	J/kg
р	Pressure	Pa.
Re	Reynolds number	
Т	Temperature	Κ
t	time	S
V_c	Curtain velocity	m/s
V_w	Window velocity	m/s
Gre	ek letters	
\dot{Q}	Volumetric flow rate	m ³ /s
a	Volume fraction	
ρ	Density	kg/m ³
μ	Dynamic viscosity	Pa – s
v	Velocity vector	m/s
σ	Surface tension	N/m

Subscripts

p, q phase index of gas and liquid respectively

v volume averaged

INTRODUCTION

Generating Bio Oil from biomass by using pyrolysis method is gaining popularity worldwide as this is from renewable resources and in contrast to other renewables, that give heat and power, Bio mass represents only source for liquid solid and gaseous fuels. Bio mass pyrolysis process provides liquid fuel that can be substitute for fuel oil in any static heating or electric generation application (A.V. Bridgewater and G.V.C. Peacock, 2000). However, its main success depends on the yield of the bio oil per unit biomass. This intern will give an idea on how economical the particular process is while producing the bio oil. Bio oil is produced by rapidly removing the heat from biomass pyrolysis vapours in heat exchangers. There are several types of heat exchangers available for the purpose. Simple indirect heat exchange can cause preferential deposition of lignin-based components leading to liquid fractionation and eventual choking in pipelines and heat exchanges (A.V. Bridgwater, 2012). Quenching in product bio-oil or in an immiscible hydrocarbon solvent is widely practised. More often quench columns are used for the purpose of condensing the pyrolysis vapours to get bio oil.

Quench columns are direct contact heat exchangers that will condense bio oil from pyrolysis vapour by removing heat from it rapidly. These direct contact heat exchangers provide cost effective heat transfer and hence it is suitable for making the process more economical and viable on commercial scale. The main idea behind this process is to get advantage of interfacial area between two working fluids in the absence of solid wall between them gives rapid heat transfer. Here it is worth noting that the rapid cooling of pyrolysis vapour is at most important as it dictates the percentage yield per biomass. Slower cooling rates encourage secondary reactions where the pyrolytic vapour compounds can crack further into smaller molecular weight fragments and/or polymerize into larger fragments, both at the expense of fragments which makeup the desired liquid product resulting to lower yield of bio oil (Diebold, J.P, 1980 and Bradbury et al, 1979). Designing quench columns using the standard empirical relations is difficult as it involves complex flow paths of the fluid inside as well as complicated heat transfer and phase change phenomena. The gas liquid interaction may generate different flow regimes, inturns determine how the fluids will behave. Hence the gas liquid interface and the effectiveness of the quench column are strongly dependent on the fluid dynamics inside the equipment. Computational methods are widely used to get extensive

understanding on the fluid behaviour inside this kind of equipment and it is necessary to design economically. The basic underlying principle on the flow regimes inside the quench column plates are very much similar to trays used in distillation columns.

Various CFD modelling studies have been undertaken to model the hydrodynamics and flow patterns in the sieve tray columns. However, according to author's knowledge no modelling attempt has been presented in the literature in modelling hydrodynamics of a quench column. This is probably due to very limited experimental data available and the very complex physics involved as mentioned before.

In this paper an attempt has been done to get information on the hydrodynamics of the fluids inside the quench column using CFD methods. Eulerian - Eulerian multiphase model with immiscible fluid option was used to model the gas liquid interactions. The CFD predictions demonstrated the flooding phenomena occurred in existing quench column design. This was observed in the experiment and was reported earlier.

The experiment conducted at Aston University was to produce bio oil based on ablative pyrolysis method (Peacocke G.V.C. et al., 1995). The detailed flow path of the process can be seen in figure 1 and experimental setup shown in figure 2. This equipment is designed to operate at 5kg/hr. throughput, but due to feeder limitation it was limited to 3kg/hr. In these experiments (Robinson, 2000), a quench column and an electrostatic precipitator were employed to condense the pyrolysis vapours to get the bio oil. The quench column is sized based on the gas flows and flooding factors.



Figure 1: Ablative pyrolysis process [US patent 7625532]

The design of the liquid collection system is as shown in figure 3. This equipment is designed for the vapour volumetric flow of $0.0011 \text{m}^3/\text{s}$ at a temperature of 400°C . The Disc and Donut within the column has the specifications mentioned in table 1. The dimensions were chosen based on curtain and window velocities calculated near the bottom of the column where maximum flow rate was expected. Correlations for these velocities are shown in equations 1 and 2. The values 1.15 and 0.58 are the recommended Souders-Brown coefficients.

$$V_{c,\max} = 1.15 \left[\frac{\rho_l - \rho_g}{\rho_g} \right]^{\frac{1}{2}} = \frac{\dot{Q}}{A_c}$$
(1)

$$V_{w,\max} = 0.58 \left[\frac{\rho_l - \rho_g}{\rho_g} \right]^{1/2} = \frac{\dot{Q}}{A_w}$$
(2)

Liquid octane at -5° C was supplied as coolant. It was reported that, at the design flow rates the quench column started flooding. This problem was rectified by lowering the flow rates of the liquid and reducing the diameter of the discs.



Figure 2: Experimental setup (adapted from Robinson 2000).

In this work, the effect of multiple chemical compounds present in the pyrolysis vapour while condensing has not been considered. As 70% of the pyrolysis product on weight basis has nitrogen which is supplied as purging as well as carrier gas, majority of the hydrodynamics effects inside the equipment were accounted. The interphase heat transfer is based on the Ranz-Marshall correlation. Some design iterations briefly discussed here and the implication of these changes on final performance also noted.



Figure 3: Sketch of the experimental quench column.

MODEL DESCRIPTION

CFD modelling

The commercial CFD package, ANSYS Fluent 13.0 was used to model the gas liquid motions in the baseline and modified quench columns. As the coolant used in the quench column was immiscible fluid, the interface area between gas and liquid is important in evaluating the fluid dynamics within the quench column. This makes the modelling more challenging. There are several methods available to trace the interface between two fluids. Among those the popular methods are volume of fluid (VOF) method and level set method. Both approaches are based on implicit free surface reconstruction methods. More recently, the immiscible fluid model for Eulerian multiphase was introduced in Fluent and is based on Geo-Reconstruct with explicit VOF option. The immiscible Eulerian model overcomes the limitation of shared velocities at the interface, present at the VOF model. In this way heat transfer modelling can be much more accurate, since a slip velocity between the different phases exists at the interface. The heat transfer coefficient between phases was calculated based on the Nusselt number using the Ranz-Marshall correlation.

The equations are as follows:

The continuity equation for the phase 'q' is

$$\frac{\partial (a_q \rho_q)}{\partial t} + \nabla \bullet (a_q \rho_q v_q) = 0$$
(3)

Note that in this problem, two phases are present, namely nitrogen (gas) and octane (liquid). Hence the conservation equations are solved for each phase individually.

Conservation of momentum yields the equation 4 mentioned below for phase q.

$$\frac{\partial (a_q \rho_q v_q)}{\partial t} + \nabla \bullet (a_q \rho_q v_q v_q) = -a_q \nabla p + \nabla \bullet \overline{\overline{\tau}}_q + a_q \rho_q \overline{g} + \overline{R} + F_{\sigma}.$$
(4)

In equation 4,

 $\overline{\overline{\tau}}_{a}$ is the stress-strain tensor,

 \overline{R} is the interaction force between two phases given by equation 5

$$\overline{R} = K(\overline{v}_p - \overline{v}_q) \quad . \tag{5}$$

Here K is the interphase momentum exchange coefficient, defined as

$$K = \frac{a_p (a_p \rho_p - a_q \rho_q) f}{\tau} , \qquad (6)$$

where f is the drag function, defined as $C_D \operatorname{Re}/24$,

and C_D is based on Schiller Naumann drag model

$$C_D = \begin{cases} 24(1+0.15\,\mathrm{Re}^{0.687})/\,\mathrm{Re} & \mathrm{Re} \le 1000\\ 0.44 & \mathrm{Re} > 1000 \end{cases},$$

$$\operatorname{Re} = \frac{\rho_q \left| \overline{v}_p - \overline{v}_q \right| d_q}{\mu_q}.$$
(8)

The term τ used in equation 6 is the particulate relaxation time and is defined as

$$\tau = \frac{(a_p \rho_p + a_q \rho_q) d^2}{18(a_p \mu_p - a_q \mu_q)} \tag{9}$$

Equations 5 to 9 are based on the symmetric model. This model is recommended when the dispersed phase in one region become continuous phase in another region of the domain. Here the subscripts p and q are interchangeable for gas and liquid based on the volume fractions.

 F_{σ} in equation (4) is the source term, which accounts the surface tension forces at the interface. The formulation for the surface tension is based on works of Brackbill et al. (1992).

$$F_{\sigma} = \sigma \frac{\rho_{\nu} k_q \nabla a_q}{0.5 (\rho_q + \rho_p)}$$
(10)

Here k_q is defined as the curvature and is computed from the unit normal which are defined as the gradient of the volume fraction of the liquid phase.

$$k_{l} = \nabla \bullet \frac{n}{|n|} \tag{11}$$

$$n = \nabla a_q \tag{12}$$

Conservation of energy for phase q gives equation 13

$$\frac{\partial (a_q \rho_q h_q)}{\partial t} + \nabla \bullet (a_q \rho_q v_q h_q) = -a_q \frac{\partial p_q}{\partial t} + \overline{\overline{\tau}}_q : \nabla v_q$$
$$-\nabla \bullet q_q + Q. \tag{13}$$

Here Q is volumetric rate of energy transfer between two phases, defined by equation 14.

$$Q = h_{pq}(T_p - T_q) \tag{14}$$

Where h_{pq} is the volumetric heat transfer coefficient between gas and liquid phases and is calculated by using the Ranz - Marshall correlation.

Geometry and mesh generation

The baseline model was constructed based on existing experimental quench column dimensions which was shown in table 1. The sketch of the experimental quench column is shown in figure 3. The original design has 18 sets of disc and donuts. Flooding is caused by choking flow near the flow area either at disc plates or donut plate's i.e.upflow of the vapour restricts the down flow of the liquid coolant (F.J.Zuiderweg, 1982). In order to assess this phenomenon in the computational model, it is sufficient to consider the bottom three stages of donut arrangement as the maximum expected flow rates of the vapour is expected in this area. For this reason, three donuts and two disc plate arrangement considered in the baseline model as shown in figure 4. Based on the observations from the results of the baseline model, a new design was proposed and is modelled. The modified design is identical to the baseline model except for the

(7)

donut plate configuration. In this model, eight holes with liners (herein after are called as caps) were placed circumferentially. This is to facilitate bypassing of some gas to next stage. The lining was about 6mm in height.

Parameters	Experiment	Baseline	
Volumetric flow rate, m ³ /s	0.0044	0.0044	
Temperature, ⁰ C	400	400	
Column diameter, cm	9.7	9.7	
Donut inner annular diameter, cm	3.4	3.4	
Disc diameter, cm	9	7.7	
Spacing between disc and donut	2	2	
Number of discs	18	2	
Number of donuts	19	3	

Table 1: Quench column design parameters.



Figure 4: Disc and Donut plate arrangement.



Figure 5: CFD Domain - Quench column.

Duo to the size of quench column (fig. 5) and its complexity of the flow behaviour, the grid size was chosen as 1.5 mm with uniform spacing. Hexahedral cells were placed inside the domain, as hexahedral mesh gives better accuracy than tetrahedral meshes while computing surface tension effects. The section of the meshed model is shown in the figure 6. Total number of cells for the baseline model is 0.66 million whereas for modified design model is 0.73 million.



Figure 6: Grid spacing - section taken at mid height.

Initial and Boundary conditions

Initially 2D models were considered as these will give quick insight into the physics. But due to flow which is highly unsymmetrical and random in nature, 3D transient analysis was adopted for this modelling task.

The initial volume fraction of coolant was set to zero and entire equipment filled with nitrogen at room temperature i.e. at 25° C. Initial velocity and pressure set to zero (gauge) in the whole domain. A mass flow rate of 0.025 kg/s of octane is supplied for the coolant inlet at -5° C. The initial run was continued until the coolant liquid reaches to the bottom surface of the equipment.

Once the liquid flow was developed, Nitrogen was injected from the vapour inlet at 400° C. The initial flow rate supplied is about 10% of the designed flow rate. Here the designed flow rate for this equipment is 0.0044m³/s, since the detailed chemical components of the pyrolysis vapours not included and the flow is assumed to be nitrogen, the calculated mass flow rate is about 0.002232 kg/s based on its density at 400°C. For the baseline model two studies conducted with different flow rates one is with 10% flow rate and another is with 50% flow rate. Whereas the modified model is run with 50, 75 and 100% flow rates respectively.

The quench column wall was considered as adiabatic and heat transfer from it is neglected. Atmospheric pressure outlet was maintained at the gas outlet. The coolant outlet is modelled as a mass flow inlet with negative flow rate. Based on the liquid levels at the bottom, the flow rate changes to either '0' or '-0.025'kg/s in order to avoid rising of the liquid coolant beyond specified levels.

RESULTS

All the models started with 0.001 s time step. After monitoring the gas temperatures at the exit and the liquid flow rate at the intermediate section which was located in between disc plate and donut, the steady state was achieved after 8s max in all cases except baseline with 50% flow case where the steady state solution is not possible due to flooding of the coolant. The presented data in this part corresponds to data obtained after this time. Figure 7 shows the coolant liquid inside the domain for the baseline case. According to the figure, the coolant liquid is clearly flowing downwards for the 10% case (50% to designed flow). It also clearly shows that in 50% flow case flooding is happening at the top donut plate as reported in the experiment mentioned earlier. The coolant liquid level is constantly rising on donut and very small quantity is flowing towards the bottom as this is evident from liquid level at the bottom for these two cases. The liquid is forced to flow upwards through the donut due to the higher pressure at the lower stages (due to rising the liquid level above the gases), however the path is blocked by choked flow of gases causing the accumulating liquid at the top of the donut further increasing the resistance of the coolant on smooth passage of the gas. This prevents the smooth flow of the coolant to the lower stages of the column and eventually leads to flooding at high gas and liquid flow rates



Figure 7: Iso-surface showing coolant in Baseline models.

Velocity vectors for the gas combined with temperature contours varying from maximum 400°C to minimum -5°C presented in the figure 8. This section created by slicing the equipment vertically at the centre which passes through the vapour inlet. From this, it can be observed that in 50% case of the base line model, the maximum velocity reached by the vapour is about 5m/s which is well below the permissible velocity mentioned in the literature based on which the equipment was designed. Since the flooding is observed at 50% flow of the designed flow itself, the 100% flow case on the baseline model was not conducted.



Figure 8: velocity vectors in Baseline models.

As observed in the figure 8, the flow is highly unsymmetrical and fluctuating from one side to the other over time. Based on the results of the baseline model, it was observed that the main issue lies with the donut plate design. The flow area for the donut plate is less than the flow area available for disc in the baseline model. In order to get same open area for disc and donut plates, eight holes with liners were introduced on donut plate. The liners on the hole ensure that only vapour will pass through these holes so that the flooding will be avoided as observed in earlier case. Figure 9 shows the coolant liquid flow pattern in the modified model for different flow conditions. From this picture it is evident that the flooding is avoided completely by this new configuration and is able to perform up to its designed limits. It was also observed that the disc plates are not holding the coolant completely and coolant is forming patterns on it. As this will reduce the heat transfer considerably, it would be better if the liners are provided for the disc plates as well so that constant level of coolant will be always maintained on the disc plates.



Figure 9: Iso-surface showing coolant in modified models



Figure 10: Velocity vectors and temperature contours in modified models.

Figure 10 shows the combined plot of velocity vectors coloured by velocity magnitude and the temperature contours for the all three cases of the modified model. From this figure it is evident that a part of the vapour is bypassing through the holes provided on the donut plates. The holes are acting as nozzles which are directing the vapour towards the disc plate. After hitting the disc plates the vapour starts circulating and flowing back towards the donut plate and contacts with coolant there by maintaining high heat transfer rate and higher effectiveness. It is also observed that the flow directions/vectors are unchanged irrespective of the flow conditions and this gives the equipment a scope for scaling up.

The average temperatures of the gas for the different cases are presented in figure 11. For the modified model at 100% flow condition, the minimum temperature attained was about 68° C which indicates that a significant amount of cooling can be achieved only by just three stages. Further cooling can be achieved if more stages are introduced inside the column. This depends on the nature of the process and the degree of cooling that is required. From this graph it is noted that major cooling is happening at disc plate interface as it presenting two types of cooling, one is impingement cooling which comes under indirect cooling and another is direct contact cooling. After passing through the holes of the donut plate the vapour is directly impinging on the disc plate which is highly desired for faster heat transfer.



Figure 11: Average temperature of the gas along the quench column height.



Figure 12: Average pressure of the gas along the quench column height. Pressures shown are gauge pressures.

Figure 12 shows the pressure plot along the length of the quench column for different runs. From this, it is clearly evident that in the baseline model 50% flow case, large pressure drop occurs at the interface of top most donut location. This is due to the increasing levels of the coolant over the vapour due to flooding. Whereas in case of 10% flow case, the maximum volume flow is occurring at the bottom donut plate level as the temperature of the vapour is high and hence the pressure drop is high at that location. In modified model cases the maximum pressure drop was limited to approximately 11 Pa as against 90Pa in the baseline case.

\CFD Run	25%	50%	75%	80%	85%		
% of inlet flow ->							
Baseline model with	8.25	-	-	-	-		
10%							
Modified model with	-	1.18	1.76	1.86	-		
50%							
Modified model with	-	0.83	1.13	1.26	-		
75%							
Modified model with	-	0.65	0.84	0.89	0.97		
100%							

 Table 2: Gas residence times (sec) inside the quench column.

The residence times for the gas flow for the different cases were tabulated in table 2. Here the top row shows the per cent of the total inlet flow which directly passing within the given time. 85% of the flow in modified model is going to outlet within 1 sec and thus rapid cooling of pyrolysis vapours can be achieved.

CONCLUSION

An Eulerian-Eulerian method with immiscible fluid model for modelling quench column hydrodynamics has been presented. The baseline model simulated for two different flow conditions, one with 25% gas flow rate and another with 50% gas flow rate. In 50% condition, flooding of the liquid coolant started on the top most donut plate as observed in the experiments. It was identified that the flow area near the donut plate is not sufficient for this magnitude of gas flow rates even though it was designed by considering the design correlations.

A modified model was developed by giving extra flow area to the gas. The results were compared against the baseline model. The modified model successfully demonstrated in handling 100% designed flow rate as well as giving better heat transfer with less pressure drop. It is also shown that in less than 1 s, the vapours can be cooled down to 77° C (temperature drop of 323° C).

Understanding of the condensation process and modeling of it can provide the detailed information on the bio oil extraction while validating with existing as well as future experiments. For this, a comprehensive condensation model is under development and results will be published by the authors in the near future.

REFERENCES

A.V.BRIDGWATER (2000), "Fast pyrolysis process for biomass", *Renewable Sustainable Energy Rev.*, **4**, 1-74.

A.V.BRIDGWATER (2012), "Review of fast pyrolysis of biomass and product upgrading", *Biomass Bioenerg.*, **38**, 68-94.

PEACOCKE G.V.C., A.V.BRIDGWATER, (1995), "Ablative plate pyrolysis of biomass for liquids." *Biomass Bioenerg.*, **7**, 147-154.

A.V.BRIDGWATER, PEACOCKE G.V.C., ROBINSON N.M. US patent number US 7,625,532.

DIEBOLD, J.P., (1980), "Preliminary Results in the Fast Pyrolysis of Biomass to Lower Olefins.", *Petroleum Chemistry division of ACS Symposium on Alternate Feed stocks for Petrochemicals*, Las Vegas, NV. USA.

BRADBURY, A.G.W., SAKAI, Y., SHAFIZADEH, F. (1979) "A Kinetic Model for Pyrolysis of Cellulose.", J. Appl. Polym. Sci., 23, 3271.

N.M.ROBINSON, (2000), "Design, Modelling and Construction of a Novel Ablative Fast Pyrolysis Reactor and Product Collection System", PhD thesis, Aston University, U.K.

J.U.BRACKBILL, D.B.KOTHE, and C.ZEMACH, (1992)," A continuum method for modelling surface tension", *J. Comput. Phys.*, **100**, 335-354.

F. I. ZUIDERWEG, 1982,"Sieve trays a view on the state of the art", *Chem. Eng. Sci.*, **37**, 1441-1464.