NEW METHOD TO DESIGN LARGE SCALE HIGH-RECIRCULATION AIRLIFT REACTORS

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Highlights:

- Fast and efficient methods are presented for designing High-Recirculation Airlift-Reactors.
- Two-phase flow of water and air is modelled.
- Improvements are made by refining steady-state models of fluid dynamics.
- Solutions are produced by varying superficial gas velocity.
- Solutions are produced by simultaneously varying down-comer and riser diameters.

ABSTRACT: High-Recirculation Airlift-Reactors (HRARs) are efficient. They use air to push a mixture around the reactor and to provide oxygen for biological micro-organisms. HRARs have been designed using programs created in the 1970s by ICI. They are limited in functionality and accuracy and need significant expert interpretation. This paper describes the creation of new structured methods that are faster and more efficient and replace the ICI methods. Models used for the calculations and the way in which they were implemented are described. The paper then describes improvements to design by analysing and improving the steady-state models of fluid dynamics within a HRAR. The models also delivered information about reactor design, especially which parameters to modify to reach a steady state result. Two-phase flow of water and air is modelled and applied to HRARs. Tests evaluated the models and some results are included. They show that varying superficial gas velocity or simultaneously varying down comer and riser diameters can create a steady-state solution. Mathematical models are used to forecast steady-state situations in the HRAR for specific gas or liquid flow rates and for various constructions. Experimental relationships forecast mass transfers between gas and liquid phases and they predict flow.

KEYWORDS

Biological reactor; Airlift; Fluid dynamics; Design program; Two-phase flow; Waste water.

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1. INTRODUCTION

The HRAR is a key component of the activated sludge water-treatment processes. It uses air to drive the waste water and to transport oxygen to biological micro-organisms in the fluid mix. A full and accurate description of HRARs can be found in [1] available from the British Library, and [2] available from Henkel AG & Company, who took over parts of ICI from AkzoNobel in 2008.

The activated sludge process has been extensively used for waste water treatment and it is effective for heavy household and industrial waste water. Airlift-Reactors are becoming more popular for producing bio-chemicals and for wastewater treatment because of their fluid dynamic characteristics [3,4]. Many research papers have described the way that the reactors depend on liquid flow, for example [5], and recent oil price increases have driven interest in understanding gas-to-liquid processes [6] but few have considered trying to improve on the main ICI design program called APRPC. APRPC has been the industrial standard program for large scale High-Recirculation Airlift-Reactors (HRARs) since it was created. Several researchers have attempted to model parts of the process [7-8] but nobody created a replacement for APRPC. This paper describes an improved replacement for that design process.

Historically, Clark performed discontinuous jar tests on the aeration of sewage in 1912, in which the resulting sludge flocs were separated from the aerated liquid and used to inoculate fresh sewage. Fowler observed these experiments and his co-workers Jones, Arden and Lockett developed experiments for a continuous flow system at Manchester in 1914. They stated that ‘failing a better term the deposited solids resulting from the complete oxidation of sewage have been designated "activated sludge"’ [Nicoll (1988)].

The activated sludge process is a form of applied microbiology that has a different objective from other biochemical processes. Other processes used a special nutrient medium and a pure culture of micro-organisms to produce an end product with certain desirable properties, as in the manufacture of alcohol and cheese. During the process, waste water is the dilute nutrient. The process is used to produce clean water and an activated sludge which represents the product in the applied microbiological sense, but which is an undesirable product usually contaminated with toxic residues.

The main components of the plant are an Aeration/Mixing System, a Reactor and a Sedimentation

Tank. The microbial biomass within the process is activated sludge, consisting mainly of bacteria and other microfauna and flora. The nutrient medium is raw sewage or other wastewater, whose concentration is expressed as a Biochemical Oxygen Demand (BOD) in mg/l, being the amount of oxygen needed to oxidise all the dissolved and suspended organic material. The working fluid is a flocculent suspension of the sludge in wastewater, and is often referred to as the mixed liquor. The normal concentration of mixed liquor expressed as Mixed Liquor Suspended Solids (MLSS) is between 2000 - 5000 mg/l.

The two stages of the process are aeration and sludge settlement. In the reactor, wastewater and recycled activated sludge are mixed and agitated. Air is added either by surface aeration or via air diffusers using compressed air. Aeration supplies oxygen to the micro-organisms in the reactor for respiration, and maintains the microbial flocs in a continuous state of agitated suspension, ensuring maximum contact between the surface of the flocs and the wastewater. During aeration, the bacteria feed on the organic matter in the wastewater converting some into new cell growth, and producing by products such as water, carbon dioxide, nitrate etc. This results in a reduction in the BOD value to 5-10% of the influent BOD. The rate of pollutant reduction is dependent upon the concentration of dissolved oxygen in the solution, and the reactor must provide a sufficiently long enough residence time for digestion of the nutrients.

Inflow of wastewater to the reactor causes mixed liquor to pass from the reactor to the sedimentation tank, in which the biomass is separated from the treated liquid. Some of the settled activated sludge in the sedimentation tank is recycled back to the reactor to maintain the microbial population at a required concentration in order to ensure continuation of the treatment. The rest is removed for further treatment and disposal. The clarified liquid, ideally free from solids, is discharged as clean effluent.

Large bio-reactors were developed by ICI to produce chemicals using AAF (aerobic airlift fermentation) technology. They were modified in the seventies to create HRAR. There is a vertical shaft in HRAR, which contains the mix of waste water. That waste water circulates because compressed air is injected and the air tends to rise and to take the waste water with it. High pressures at depth lead to a high concentration of dissolved oxygen, and that in turn leads to significant increases in the rates of chemical and biological reaction. The vertical shaft is typically 50 to 150m deep in the ground and is about one to six metres in diameter. It is separated into down flow and up flow segments, called the “down comer” and “riser”. The “down comer” and “riser” connect at the lowest point to create a very large "U" tube. A

holding tank sits at the top of the reactor. Liquid can be drawn into the down comer from the holding tank and liquid ascending the riser can return to the tank after treatment. The large "U" tube in the ground is an effective replacement for the more usual shallow aeration-basins within more conventional processes.

The advantages of HRAR are:

- Reduced land usage; *HRAR uses less than a quarter of the land covered by conventional plants of similar capacity (and it can be as small as 10%). That means HRARs can be built in areas or countries where there is little land available for industrial or wastewater treatment use. There is also less disturbance to the environment and can be a reduction in capital costs and initial outlay.*
- Reduced power; *HRAR processes use a quarter of the power used by more conventional plants. It is an effective system that can achieve 3 - 4 kg BOD/kWhr.*
- Lower environmental impact; *HRARs are less damaging to environments than more conventional plants. There is also a significant reduction in smell, noise, mists and sprays.*
- High performance; *Because of the depth of the "U" tube, reactions take place with higher oxygen transfer rates so that higher strengths of waste water can be treated successfully.*

The structure of a HRAR is illustrated in Figure 1

Figure 1 here. A High-Recirculation Airlift-Reactor

Air can be initially introduced into the riser to start fluid circulating in the "U" tube (the "airlift" principle). Once the fluid is circulating, wastewater can be introduced and air can also be injected into the down comer of the HRAR. That air is pulled downwards with the circulating waste water to the bottom of the "U" tube reactor and then up the riser. Air creates a void fraction and reduces average density within the riser compared to un-gassed waste water in the down comer that is still above the air injection point. This creates the flow in the "U" tube reactor.

In addition to inducing the flow, the injected air provides oxygen for the bio-chemical processes. Very high pressures at the lowest part of the "U" tube reactor forces oxygen into solution so that it is readily accessible to micro-organisms in the waste water. High concentrations of dissolved oxygen at the

bottom of the reactor make it an ideal environment for micro-organisms.

The main idea of the research described in this paper was initially to improve the design process and then to reduce running costs and construction costs by eradicating some needless conservatism from the process of design. There are more than sixty HRAR plants operating world-wide, often handling far more wastewater for more diverse industries than was ever considered during design. There was clearly slack in the design process. In addition, a HRAR can cost about £15 million. Excavation costs to sink the deep "U" tube are a substantial part of the construction cost and reducing the depth or size of the "U" tube would deliver generous savings. The cost of running a HRAR can be about £300,000 per year and improving design could substantially reduce that cost.

As an example, Anglian Water has the biggest HRAR at Tilbury in England and it was designed with the ICI programs. The plant was planned to treat waste water equivalent to that produced by just over three hundred thousand people within an area of only 20,000 square meters (two hundred by one hundred metres). The HRAR consistently and efficiently treats more than 2.5 times the planned loading. This demonstrates that the programs underestimated the process performance, causing increased capital cost to the customer and, potentially, loss of market to the designers.

The main design work for HRAR was conducted in the late seventies by ICI. They called it "Deep Shaft". The software used in the design of HRARs was in FORTRAN (Fields, 1991). These had little structure and when they were investigated and dissected, it was difficult to understand the processes that parts of the programs were performing. This prevented effective development and study. A decision was made to write new design programs from scratch.

An HRAR has two separate but interrelated aspects to it. Firstly there are the biological processes. They reduce organic matter within the waste water. Secondly fluid dynamics calculations are required to explain the complicated two-phase flows within the "U" tube. These two aspects are connected by the precipitation rates and solution of gas (es).

Initially, to start the fluid circulating in the shaft, air is only inserted in the riser. Bubbles create a voidage as the air ascends, reducing mean density of fluid over the place where the air was injected. Hydrostatic drive is created in the shaft, as fluid in the down comer has zero or very low voidage. Once the liquid flow rate has reached a threshold level, air is gradually swapped from the riser to the down

comer to make the air available for the maximum amount of time. The air in the down comer is pulled to the bottom of the "U" tube by the fluid. In doing so the pressure increases and the air dissolves, reducing the voidage. After passing the bottom turn into the riser, gases precipitating in the reducing pressure field create bubbles, which drive the flow up the riser. That makes the system more complicated because that introduces instability. If the liquid velocity in the down comer becomes less than the velocity of the bubbles rising [9], gas will accumulate in the down comer and the flow will reverse, with potentially violent consequences. As more air is transferred to the down comer, more and larger (faster-rising) bubbles appear in the down comer, and the stability of the system decreases.

The new programs described in this paper use mathematical models to forecast steady-state conditions in the "U" tube for specific gas or fluid flow rates and for various HRAR constructions. Empirical correlations forecast the transfer of masses between the gas and fluid phases throughout the "U" tube [10] and they predict flow [11,12]. The research described here did not consider operating transients or control systems as it was intended to improve the prediction of steady state performance at the design points. First, a new design program was created that operated faster and more efficiently than the ICI design programs then that program is improved to produce better designs.

2. A NEW DESIGN PROGRAM

The new design program could run in two design modes: "general" or "specific".

The general design mode was used when a new reactor was to be designed. Calculations were performed using input data that specified the design criteria in terms of process performance, reactor geometry, biological kinetic factors and dynamic performance factors. From this specification, the new design program calculated injection depths, air rate, liquid volume flow rate and other related parameters, such as the process oxygen efficiency.

The specific design mode was used to modify an existing design solution in order to determine the performance of different reactor configurations. In this mode, the user specified values for the air input rate and injection depth, along with a range of liquid flow rates for which the new design program calculated the excess drive and the output BOD.

The principal design criteria defined the required effluent discharge standard, primarily stated as a limit on BOD and concentration of Suspended Solids (SS). The SS criterion is achieved by downstream processes, and is not considered further. The new design program calculated the oxygen input rate necessary to cause the BOD reduction required to achieve the output standard. This value, which was a constant, was then compared with the quantity of oxygen calculated to have been transferred to the organisms, and iterative calculations were performed until the difference between the two values was within a pre-defined tolerance.

On the down comer, air was injected into a vertically downward fluid flow and was drawn down by the flow, overcoming the air's natural tendency to rise. The velocity of the flow therefore had to be greater than the rise velocity of the air bubbles. The gas void fractions in the reactor were also dependent on the flow velocity and these determined the driving force for fluid flow in the reactor so that drive criteria and stability needed to be considered when generating the solution. The new design program dealt with these requirements using the following logic:

- i) *If OXYGEN TRANSFER was insufficient then the AIR INPUT RATE was increased.*
- ii) *If STABILITY MARGIN was not satisfied then the LIQUID CIRCULATION VELOCITY was increased.*
- iii) *If DRIVE was insufficient then the INJECTION DEPTH was increased.*

Figure 2 is a simplified diagram outlining the general design mode.

The air input rate to the down comer sparger was initially set to equal the air input rate calculated as being necessary to remove the required BOD. A 100% transfer efficiency was assumed, which ensured that this figure was an underestimate, which in turn ensured rapid convergence of the oxygen transfer requirements. Air could also be added in the riser. Riser air increased the drive because it increased the gas void fraction in the riser and decreased the quantity of air required for BOD removal in the down comer. However, this air was used less efficiently by the reactor, as the contact time with the micro-organisms was less than for the air input in the down comer.

Liquid volume flow rates were chosen and calculations performed to find the injection depths corresponding to each of these volume flow rates. The results were fitted to a parabolic curve to provide a characteristic equation of injection depth against the liquid volume flow rate for the reactor. A stability

criterion could then be applied to find the operational po

The injection depth and gas transfer calculations were performed in a loop around the reactor. Concentrations were assumed for Oxygen, Nitrogen, Carbon Dioxide and the BOD for the circulating liquor at the top of the down comer. int at the apex of the curve.

Figure 2 here. Simplified Logic Diagram for the General Design Mode

The reactor was divided into sections and hydraulics and gas transfer calculations were performed in each of these sections in a loop around the reactor. Iterative calculations were performed at the end of a loop and the loop was repeated until the concentration figures converged within pre-defined tolerances.

Once the operating point had been located, the oxygen transfer was checked and adjusted if required. The complete cycle of calculations was repeated until a design solution was achieved. Finally the results were output to a data file.

When operating in the specific design mode, the oxygen transfer and stability iterative calculations were not performed. The concentration calculations and iteration cycle were performed for each of the stipulated liquid volume flow rates.

Characteristic design curves could be plotted by drawing a graph of injection depth against air input rate. These defined the region within which a possible design solution lay. The constraints imposed on the system were twofold. For a given injection depth, if the air input rate was too low then the result was insufficient oxygen transfer. For a given air input rate, there was a minimum injection depth above which the system would become unstable. This is shown in Figure 3.

Figure 3 here. HRAR Operating Zone

For a design to have been feasible, it had to lie within the unshaded area between the two curves. This meant that as well a minimum air rate, there was also a maximum air rate beyond which the gas void fractions on the down comer would become excessive, resulting in an unstable system.

2.1. The Construction of the new program

The new software was created in VISUAL BASIC. It was made up of a controller module and twenty six sub modules. A module *Setup* read the input data from a data file and created a results output file. Parameter values were converted to standard SI units and reactor geometry calculations were performed by a *Preliminary* module, followed by an *Initialise* module which initialised the system design parameters and calculated the mass transfer coefficients and Henry's constants values.

Key modules within the new design program controlled specific aspects of the design process and executed other modules in sequence. Two distinct paths were established in the controlling module *Main*, one each for the general and specific design modes.

The detailed structure of the new design program can be made available on request.

2.1.1. The General Design Mode

This was the main mode of operation in which a full solution was developed. The down comer air input rate and depth of injection weren't defined at input. If riser air injection was required then the air input rate and depth of injection had to be specified. In the *Main* module, two modules were executed within a loop which was repeated until the oxygen transfer requirements had been satisfied. The first of these was *Define_Curve* which calculated the characteristic curve of fluid flow rate against the depth of air injection by specifying fluid flow rates and executing *Shaft_Circuit* to calculate the corresponding injection depths. Once the curve had been defined and the nose located, *Locate_Point* calculated the operating point by application of the stability criterion relative to the nose of the curve. This gave a solution in which drive and stability requirements were satisfied. Operation then returned to *Main*, where the gas void fraction at the down comer sparger was checked to see whether it exceeded the critical value. The void fraction was checked at the down comer sparger, as this was the point of highest gas void fraction on the down comer. If the critical void fraction was exceeded, then a warning message was generated and execution continued. The oxygen transfer was then checked by *O2_Iteration*, which updated the oxygen and nitrogen input values at the down comer sparger if the value of oxygen transferred was not within one per cent of the value required. If the oxygen transfer values had started to diverge then the gas input rates before the

divergence were carried forward, a warning was generated to indicate this condition and the iteration process was stopped.

2.1.2. The Specific Design Mode

In the specific design mode the depth of injection in the down comer and the air input rate were specified at the start, along with a series of superficial fluid velocities. The new program calculated the reactor performance for each of these velocities. The liquid volumetric flow rate was calculated from the superficial liquid velocity and then *Shaft_Circuit* was executed to calculate the drive at this flow rate, noting that the injection depth remained constant. The results were output to a data file and the cycle was repeated for each superficial liquid velocity value.

2.2. Calculation Theory and Implementation

Before the design process could begin the input data specifying the design criteria had to be converted into the required parameters and some initial calculations performed.

2.2.1. Initial Calculations

Parameter values were converted to standard SI units and reactor geometry calculations were performed in *Preliminary*. These included the riser and down comer cross sectional areas, the reactor diameter and the hydraulic diameters. For the case of a partitioned reactor, the down comer area share was used to calculate the angle of a sector that would represent this area fraction. This value was then used in the calculations for overall reactor diameter and the hydraulic diameters. *Initialise* initialised the HRAR design parameters and calculated the mass transfer coefficients and Henry's constants values.

The initial air input rate at the down comer sparger was set to equal the air rate required to remove the specified BOD; this calculation assumed a 100% transfer efficiency. This assumption ensured that the air input rate was an underestimate which increased the convergence rate of the oxygen transfer value. This can be illustrated by considering a case where excess air had been specified. The air input rate

adjustment was accomplished by multiplying the current value by an air adjustment factor. The air adjustment factor was calculated by dividing the oxygen transfer required by the oxygen transfer calculated for the current air input rate. If the oxygen transfer was limited by the biological kinetics then the air adjustment factor would be less than that required to minimise the air input rate, even though the required BOD removal had been achieved due to the excess air.

The air input rates were converted into oxygen and nitrogen flows of kgmol s^{-1} . This eliminated problems associated with pressure, volume, temperature and gas composition, all of which were constantly changing. The molar flow rates remained constant, thus simplifying the flow calculations. The gas flow rates were given by:

$$\dot{m}_{\text{Gas}} = \dot{m}_{\text{N}_2} + \dot{m}_{\text{O}_2} + \dot{m}_{\text{CO}_2} \quad (1)$$

$$\dot{V}_G = \frac{\dot{m} \times R \times T}{P} \quad (2)$$

Initial values were set for the BOD and gas concentrations and the gas flow rates were set to zero. First estimates of the injection depth in the down comer and fluid flow rate were set according to the following criteria:

$$\text{Injection Depth} = (\text{Reactor Depth})^{0.75} \quad (3)$$

$$\dot{V}_L = \frac{0.6 \times \text{Process Volume}}{\text{Reactor Depth}} \quad (4)$$

The initial estimate of the liquid volume flow rate was set such that the down comer liquid velocity was of the order 1.5m/s. The process volume divided by the reactor depth gave the total reactor area. The down comer area was generally of the order $0.4 \times$ reactor area; dividing this into the reactor area calculation gave the liquid velocity, as the reactor areas cancelled. This liquid velocity was only an estimate as it did not account for the air content and the liquid velocity varied around the reactor. The mass transfer coefficients were calculated at 20°C using the modified equations of Calderbank and Moo Young [13]:

For bubbles smaller than 2.5mm diameter:

$$MT = 0.31 \times KS \times \left(\frac{g \times \mu_v}{\rho}\right)^{\frac{1}{3}} \left(\frac{\rho \times D}{\mu_v}\right)^{\frac{2}{3}} \quad (5)$$

For bubbles larger than 2.5mm diameter:

$$MT = 0.42 \times KL \times \left(\frac{g \times \mu_v}{\rho}\right)^{\frac{1}{3}} \left(\frac{\rho \times D}{\mu_v}\right)^{\frac{1}{2}} \quad (6)$$

The parameters *KS* and *KL* were correction factors taken from ICI which were set at 0.6 and 1 respectively. These factors had been established by ICI from HRAR design trials [ICI (1991)].

A temperature correction factor was applied to the mass transfer coefficients to give values at the reactor temperature [14]:

$$MT = \text{COEFFICIENT}(@20^\circ\text{C}) \times 1.024^{(T-20)} \quad (7)$$

The Henry's constant parameters were derived as linear functions of temperature between 0 and 35°C for oxygen and nitrogen:

$$HN = HC \times 10^7 \times \left(\text{COEF1} + \text{COEF2} \times \frac{T}{35}\right) \quad (8)$$

For carbon dioxide the temperature effects were more pronounced and consequently two equations were used, one applicable between 0 and 20°C (Eqn. 9) and one from 20 to 35°C (Eqn. 10):

$$HN = HC \times 10^6 \times \left(\text{COEF1} + \text{COEF2} \times \frac{T}{20}\right) \quad (9)$$

$$HN = HC \times 10^6 \times \left(\text{COEF3} + \text{COEF4} \times \frac{T - 20}{15}\right) \quad (10)$$

2.2.2. Stability

Stability calculations were only performed when the new program was operating in the general design mode because they required modification of the injection depth in the down comer, which was an input when in specific design mode. *Define_Curve* determined the characteristic curve of fluid flow against the depth of injection in the down comer. Three fluid flow rates were carefully chosen. They ranged from 0.2 x the reactor

area to $0.8 \times \text{reactor area}$ [12,13]. That provided a series of fluid velocities from about 0.5 ms^{-1} to 2 ms^{-1} ; the normal range that produced a functioning design. If the fluid velocity in the down comer was below $1.5 \times \text{bsv}$ (bubble slip velocity), fluid velocity was fixed at $1.5 \times \text{bsv}$. If this happened for all 3 fluid flow rates that were selected to locate the characteristic curve then the software paused. An error message was then produced to say that it was not possible to create a stable scheme with the proposed reactor shape and arrangement.

Shaft Circuit was executed to calculate the down comer injection depth corresponding to each of the fluid flow rates. The down comer sparger gas void fraction at the center of the three rates was presumed to be an apex of the characteristic curve [11]. This was kept to be exploited later in *Locate Point* so that the stability criterion could be applied later. Fluid flow rates were tested against bsv again, and if the criteria was met then the design program stopped because a parabola could not be fitted to describe the characteristic curve.

Parabola fitted a parabolic curve to the solutions to produce a specific equation. Initial parabolic curve coefficients were stored to match the operating point [11]. Fluid flow at the curve apex was determined. That was achieved by differentiating the curve equation and equating it to zero. The quantity obtained was evaluated against the center of the 3x fluid flow rates used to create the curve to test if it was inside a stipulated variance. If it was not then the range of the 3 x fluid circulation rates was employed to find the representative specific equation. The procedure was recurrent and so the procedure repeated. If fluid rates at the apex diverged then preceding results were taken forward.

Locate_Point determines the operating point after the apex has been found. The curve,

$$Y = a (x)^2 + b (x) + c$$

was computed from the original three circulation rates and was employed in calculating depth of injection at the apex [11,12]. It was then possible to apply the stability criterion to locate the operating point relative to the apex.

$$\text{Stability Margin} = (I_{OP} - I_{AP}) \times \mathcal{E}_{SPARGER@APEX} \quad (11)$$

Injection depth could then be placed into the equation to give two fluid flow rates.

Figure 4 here. Characteristic Curve of Fluid Flow against depth of injection

The new program guaranteed that the bigger of the flow rates was chosen, as that would be stable (Fig. 4). Figure 4 shows the curve with a depth of injection quantified along with the two associated fluid flow rates. Considering the greater of the flows, Point A, if a disruption caused an increased fluid flow rate, the depth of injection would need to be increased in order to uphold that higher rate. In other words an increase in the drive would be required. The depth of injection was constant for a particular configuration so more drive couldn't be provided and the reactor slowed to the earlier fluid flow. If the fluid flow decreased then a surplus of drive within the reactor tended to increase fluid flow. So, at the higher fluid flow, it has some self-correcting features.

At the lower fluid flow, Point B, if the analysis is performed again then the drive characteristics would mean the reactor was unstable. In other words, any disruption to fluid flow is compounded.

2.2.3. Concentration and Drive Calculations

These calculations were performed by dividing the reactor into sections and analysing one section at a time. This was controlled by *Shaft_Circuit*, which calculated the injection depth corresponding to a given liquid volume flow rate. In the specific design mode *Shaft_Circuit* also calculated the excess drive at various liquid volume flow rates for a given injection depth and air input rate.

The reactor was divided into a number of sections and analyses were performed sequentially around the reactor from the top of the down comer to the top of the riser. Calculations were performed to determine gas concentrations and the pressure profile around the reactor, from which the net drive could be determined. These consisted of calculations for gas void fraction, mass transfers, biological kinetics, pressure and frictional losses.

The first calculations performed addressed the mass transfers in the head tank as a circuit finished at the top of the riser. These calculations were not performed on the first circuit, as values for the gas flow rates and partial pressures, which were required for the calculations, were not available until a reactor cycle had been completed. The head tank was not included in the first cycle of the reactor because the wastewater entered the reactor after the head tank, directly into the down comer and so the initial concentration values could only be applied in the down comer.

The initial gas concentrations were calculated at the top of the down comer. These concentrations were

calculated from the influent, the returned activated sludge and the circulating liquor flowing into the first section. On the first circuit these concentrations were set in *Initialise*. The running totals of O₂ removed, CO₂ produced and pressure drops were set to zero.

Voidage determined the gas void fraction in each section. From this the gas volume in the section was calculated and the total bubble surface area. The gas partial pressures were calculated and used to find the mass transfers, which were checked to ensure they were not greater than the gas molar flow rates. The new molar flow rates were then determined. On completion of the gas transfer calculations *Kinetic* calculated the BOD removal, oxygen uptake and CO₂ production.

The drive calculations were the final sectional calculations and included pressure, frictional losses, and gas void fraction and hydraulic head calculations. The frictional pressure drop was calculated in *Friction* using a modified Darcy equation.

Once the calculations had been completed for the current section, the following section was examined to see if an air input sparger would occur before or at the bottom of that section. If so, then the appropriate air input module was executed (*Pre_Dcomer_Sparger* for the down comer, *Pre_Riser_Sparger* for the riser). At the bottom of the reactor and the top of the riser the modules *Bottomturn* and *Topturn* applied a secondary pressure loss term to account for the turning of the flow of the form:

$$\text{PRESSURE}_{\text{loss}} = 4.f.\frac{1}{d}.\frac{\rho u^2}{2} \quad (12)$$

(from [15]).

Once all the reactor sections had been examined, *Converge* performed the iterative calculations on the gas and BOD concentrations and the injection depth. *Converge* was structured so that each parameter was checked in turn. If any parameter required adjustment, the adjustment was made and a new reactor circuit commenced. The injection depth adjustment was calculated from the net pressure change around the reactor. Convergence was reached when this net pressure change was zero.

2.2.4. Sectional Calculations

The following Sections describe the calculations performed for each reactor section. With the exception of the

air injection calculations these were performed for every section of the reactor.

(a) Gas Void Fraction Calculations

The gas void fraction was calculated from the liquid and gas flow rates and the slip velocity. Experiments had demonstrated that when the gas void fraction was above some critical value, the bubble slip velocity varied with gas void fraction, gas superficial velocity and liquid superficial velocity due to bubble coalescence [14,16]. If the gas void fraction was below this critical value, set at 0.2 (20% gas by volume) then the slip velocity was assumed to be constant. The slip velocity was set as an input parameter, normally at 0.24m/s. The gas void fraction was calculated using one of two equations, one of which only applied when the gas void fraction in the riser was greater than the critical value. It was assumed that the gas void fraction on the down comer would not exceed this critical value and so the following equation was used

$$S = \frac{\dot{V}_L}{A(1 - \varepsilon)} - \frac{\dot{V}_G}{A \times \varepsilon} \quad (13)$$

If the gas void fraction in any riser section was above the critical value then a second equation was applied as follows [14]:

$$\frac{V_G}{\varepsilon} = S_{CRIT} + PARAM1(V_G + V_L)^{PARAM2} \quad (14)$$

The two parameters in this equation were specified in the the program input data file. The recommended values from ICI were 1.20 and 1.0 respectively [14,17].

(b) Mass Transfer Calculations

The mass transfer calculations were performed after the gas void fraction and gas volume calculations had been completed. The number of bubbles flowing was assumed to remain constant until the next air input point and so was only calculated in the first section in the down comer and at an air input point [18].

$$BF = \frac{6 \times \dot{V}_G}{\pi \times BEQ^3} \quad (15)$$

The bubble diameter was calculated for each section:

$$BEQ = \left(\frac{6 \times \dot{V}_G}{\pi \times BF} \right)^{\frac{1}{3}} \quad (16)$$

The number of bubbles in each section was given by:

$$BN = \frac{A \times L \times \varepsilon \times BF}{\dot{V}_G} \quad (17)$$

Thus the total surface area for gas transfer was calculated from:

$$BA = BN \times \pi \times BEQ^2 \quad (18)$$

The partial pressure of each constituent of the gas phase was calculated as shown below for oxygen:

$$PARTP = \frac{\dot{V}_{O_2}}{\dot{V}_G} \times P \quad (19)$$

Utilising the coefficients calculated in *Initialise*, the mass transfers of each gas from bubbles to the liquid were determined using the standard mass transfer equation:

$$\text{Mass Transfer} = C1 \times C2 \times BA \times \left(\frac{PARTP}{C3 \times C4} - \text{Gas Concentration} \right) \quad (20)$$

The coefficients C1 and C3 were correction factors for the mass transfer coefficients and Henry's constant from the clean water value for the mixed liquor and were defined as follows [17]:

$$C1 = \frac{MT_{\text{mixed liquor}}}{MT_{\text{clean water}}} \quad (21)$$

$$C3 = \frac{HN_{\text{mixed liquor}}}{HN_{\text{clean water}}} \quad (22)$$

(c) Biological Kinetics Calculations

The rate of BOD removal, oxygen uptake and carbon dioxide production were determined by the module *Kinetic*. The quantity of BOD or substrate removed was calculated using a Monod type equation as shown in Equation 23. K1 and K2 were the kinetic constants and were input parameters. These could be determined from fermenter trials, pilot plant tests, or from a previous plant with similar effluent. If none of these sources

were available then suitable values could be taken as specified in Table 1, based on an MLSS value of 5 g/l.

$$\text{BOD Rem. Per Sec.} = \frac{K1 \times \text{MLSS} \times A \times L \times (1 - \varepsilon) \times \text{BOD Conc.}}{(1 + K2 \times \text{BOD Conc.})} \quad (23)$$

Table 1 here. Kinetic Constants

Provided that the correct Food:Mass (F:M) ratio (the ratio of the weight of BOD applied each day to the unit weight of activated sludge under aeration) had been selected then the consequences of specifying incorrect kinetic constant values were generally not serious because:

- 1 If K1 and K2 were set too low then the program could not generate a solution because the biological kinetics could not remove the BOD load in the given reactor volume.
- 2 If K1 and K2 were set too high then the principal change was in the BOD and oxygen profiles around the reactor. Due to the increased biological activity predicted by the higher constants, the oxygen concentration would become limiting earlier and consequently would equal the minimum value over a much larger range of the reactor profile. Oxygen transfer would be over-predicted as a result because the concentration was a factor in the transfer equation. This effect would only be slight, as the equilibrium dissolved oxygen over most of the reactor circuit was large compared with the actual dissolved oxygen. The designer could evaluate the significance of any over-estimate of the kinetic constants by examining the range over which the dissolved oxygen concentration was at the minimum value.

The rate of oxygen uptake was determined by multiplying the BOD removed value by an oxygen to BOD ratio. This assumed that there was enough oxygen to meet the biological requirements, that is, that the rate of BOD removal was limited by the biological kinetics. A minimum dissolved oxygen concentration was specified in the input data, below which it was assumed that there was insufficient oxygen available for the biological activity to take place. The oxygen concentration was checked to see if this minimum value had been reached. If so, then the oxygen concentration in the section was set to this minimum value and the oxygen uptake and BOD removal values recalculated to suit.

The carbon dioxide removal rate was calculated by multiplying the oxygen removal rate by a carbon dioxide to oxygen ratio. This calculation was signed negative as it was calculating the carbon dioxide

produced by the respiration of the biological organisms utilising the oxygen to consume the BOD. That is, it is not actually a removal rate but a rate of production.

Finally, the new BOD concentration was calculated and the total oxygen and carbon dioxide removal rates incremented by the values from the current section. The total removal rates were the sum of all the rates from each of the sections around the reactor, as the reactions were occurring concurrently throughout the reactor.

(d) Frictional Calculations

These were performed in *Pressure*. The Reynolds number for the flow was calculated and the friction factor was then found by iteration of the following equation [19]:

$$FR = 2 \left\{ -2.5 \ln \left(0.27 \times \frac{k}{HDIA} + \frac{0.885}{RN} \sqrt{\frac{2}{FR}} \right) \right\}^{-2} \quad (24)$$

The friction factor was then substituted into the Darcy homogeneous flow equation to determine the pressure drop due to friction in the section:

$$\Delta P = 4 \times FR \times \frac{L}{HDIA} \times \frac{1}{2} \times \rho_L (1 - \varepsilon) \left(\frac{\dot{V}_L}{A} \frac{1}{(1 - \varepsilon)} \right)^2 \quad (25)$$

This equation was modified to account for the gas by factoring the liquid density by one minus the gas void fraction and calculating the actual liquid velocity.

The section gas void fraction and hydraulic heads were calculated as follows:

$$\text{Gas Void Fraction Head} = \rho_L \times g \times L \times \varepsilon \quad (26)$$

$$\text{Hydraulic Head} = \rho_L \times g \times L \quad (27)$$

Thus the pressure at the top of the following section could be evaluated:

$$P = P - \Delta P + (HH - \varepsilon H) \times SW_D_R\% \quad (28)$$

(e) Air Injection Calculations

Separate modules were used for calculating the air input in the down comer and in the riser, though both modules were of the same construction. If the injection depth did not occur at the start of a reactor section, then the section within which the air input point occurred was divided into two smaller sections so that the air was

input at the start of one of these smaller sections. In order to achieve this the air injection calculation modules (*Pre_Dcomer_Sparger* for the down comer, *Pre_Riser_Sparger* for the riser) had four sub-sections.

If the injection depth was at the start of the following section then the first sub-section added the air. If the injection depth was at the bottom of the following reactor section then the second sub-section set a flag to indicate that air injection was to occur one interval later. The third sub-section reset the reactor section length and recorded the gas void fraction and pressure at the sparger after the air input calculations had been performed. The final sub-section was executed when it became necessary to reset the section length in order to ensure that the injection point was at the start of the next section.

The bubble equivalent diameter was calculated at the air input point:

$$BEQ = \frac{(N2A + O2A) \times BEQS + (\dot{V}_{N2} + \dot{V}_{O2} + \dot{V}_{CO2}) \times BEQ}{N2A + O2A + \dot{V}_{N2} + \dot{V}_{O2} + \dot{V}_{CO2}} \quad (29)$$

The input gas flows were added to the existing gas flow values to give the new gas flow rates and the number of bubbles flowing per second was recalculated:

$$BF = \frac{6 \times \dot{V}_G}{\pi \times BEQ^3} \quad (30)$$

2.2.5. Head tank Calculations

The head tank was a functioning part of the reactor and as such mass transfer and biological kinetics calculations were performed. The principal function of the head tank was to dispel the gases from the fluid flow. The assumption was made that the gas was dispelled evenly in each section of the head tank. In order to model this the gas flow rates were reduced in each section until a pre-defined gas entrainment percentage value was reached. The entrainment value was a statement of the amount of gas remaining in the fluid leaving the head tank and was a volumetric criteria specified as an input criteria.

The head tank was divided into a number of sections, as specified in the input data. The cross sectional area of each head tank section was set to 1m² so that the section length was determined by dividing the head tank volume by the number of sections. The gas entrainment was specified in the input data as a fraction of the gas volume flow into the head tank (normally 0.05 ie. 5% entrainment). An entrainment factor was calculated so that an equal quantity of gas was expelled in each section:

$$\text{Entrainment Factor} = \text{Gas Entrained}^{\left(\frac{1}{\text{NS}}\right)} \quad (31)$$

The sectional calculations were set within two loops. The outer loop checked that the gas volume flow rate exiting the head tank was less than the assumed entrainment value, and if not, added sections on to the head tank until this requirement was satisfied. The inner loop performed the calculations for each section. The gas void fraction, the number of bubbles flowing and the total surface area for gas transfer were calculated. The mass transfers were then calculated, for which there were different calculations depending on the bubble size. The mass transfer values were checked to ensure that they were not greater than the gas flow rates and *Kinetic* was executed to calculate the BOD removal, oxygen uptake and carbon dioxide production. The new gas concentrations, gas flow rates and total gas flow rate were calculated and the sequence repeated for each section.

2.2.6. Air Input Rate Calculations

On completion of the calculations to determine the down comer injection depth *O2_Iteration* calculated the down comer air input rate. The calculated value of oxygen transferred summed for all the reactor sections was compared with that necessary to remove the required BOD. If these values were not within tolerance, set at one per cent, the oxygen transfer value was compared with that from the previous circuit to check for divergence. If divergence had occurred, then preceding results were taken forward. If the oxygen transfer value had not diverged then the air rate was reset:

$$\text{O2A} = \text{O2A} \times \frac{\text{O2R}}{\text{O2REM}} \quad (32)$$

The nitrogen input rate was adjusted to suit the new oxygen input rate:

$$\text{N2A} = \text{O2A} \times \frac{(1 - 0.2095)}{0.2095} \quad (33)$$

where: 0.2095 = O₂ fraction in air

3. FINAL DESIGN CALCULATIONS

After completion of the iterative design cycle, final calculations were performed by the module *Design*. These

included: conversion of units; efficiency calculations, such as that of oxygen utilisation and the percentage of the BOD removed.

The oxygen intensity, an indication of the quantity of oxygen used per unit volume of flow per hour, was calculated accordingly:

$$\text{O2 Intensity} = \frac{\text{O2 Removed Per Hour}}{\text{Process Volume}} \quad (34)$$

The gas and liquid superficial velocities were calculated for the reactor, the down comer and the riser [20]. To calculate the reactor gas superficial velocity, all the air was assumed to be added at the down comer. The form of the calculations was as shown:

$$V_G = \frac{\text{Air Added}}{A} \quad (35)$$

The riser gas superficial velocity was calculated by dividing the down comer value by one minus the down comer area share. The superficial liquid velocities were calculated from:

$$V_L = \frac{v_L}{A} \quad (36)$$

The velocity head losses in the main sections of the down comer and the riser [21] were calculated from:

$$\text{VLD} = 0.5 \times \left\{ \frac{\text{Total DComer. } \Delta P}{0.5 \times \rho_L \times V_{Ld}^2} - \text{VLB} \right\} \quad (37)$$

When a partitioned reactor was specified, the centre angle of the chord of the partition wall was determined by iteration of an equation defining the chord centre angle in terms of the down comer area share:

$$\theta_n = \pi \times (0.5 - \text{DAS}) - 0.5 \times \text{SIN}(2 \times \theta_{n-1}) \quad (38)$$

This calculation was derived from examining the reactor area share as a segment and a corresponding sector, as shown in Figure 5. The areas of the sector OAC and the triangle OAC were calculated in terms of the angle θ and the area of the circle.

Figure 5 here. Partitioned Reactor Areas

The area of the triangle was then subtracted from the area of the sector and equated to the down comer area

fraction. This was then rearranged to give the equation above in terms of the angle θ . The chord angle was then used to determine the riser and down comer hydraulic diameters:

$$\text{Downcomer Hyd. Diameter} = \frac{2 \times \text{DAS} \times \pi \times D}{2 \times \cos \theta + \pi - 2 \times \theta} \quad (39)$$

$$\text{Riser Hyd. Diameter} = \frac{2 \times (1 - \text{DAS}) \times \pi \times A}{2 \times \cos \theta + \pi + 2 \times \theta} \quad (40)$$

The final results were then output under the following sections: Drive data; Reactor geometry; Process data; Hydraulic data; Air supply data; Parameters at the characteristic nose; Iteration counts.

4. EVALUATION OF THE NEW PROGRAM

The new design program has been tested using input data sets for HRARs used with the original ICI steady state design program. After several extensive debugging sessions, the new program consistently produced results that were within approximately 0 to 2% of those obtained using APRPC.

More importantly, the new program was faster, easier to use and is therefore potentially more efficient. The original ICI design programs took hours to run one set of calculations (often left overnight to complete them). After a set of calculations the program would stop and wait for new instructions. Human operators then inspected the outputs and revised their inputs in an attempt to find a working solution. Then they ran the program again and waited (or more likely worked on something else) until it was done.

The new program was much faster and automatically adjusted new inputs depending on previous outputs.

5. IMPROVING THE NEW DESIGN PROGRAM

The new program was constructed from an investigation of previous research concerning airlift reactors. The research presented in this paper assumed that:

- Water was the fluid phase.
- Water could not be compressed for pressure ranges within an HRAR.
- Down comer voidage fraction $\epsilon_d = \text{Zero}$. Based on: (1) Gas being injected at the bottom of the riser, and

(2) An assumption that total gas separation happened within a separation tank.

- Riser voidage fraction ϵ_r remains the same. This simplified modelling but was incorrect as it required a constant riser pressure. Riser superficial fluid velocity ($V_{Lr} = \text{volumetric flow rate} / \text{reactor area}$) assumed the fluid was water. V_{Lr} was constant in the riser. It interrelated with V_{Ld} by a ratio of area for the riser to area for the down comer. If they had the same cross sectional areas then $V_{Ld} = V_{Lr}$. The interstitial liquid velocity U_L within the riser and down comer would be different.

The first simulation was similar to a model by [1], based on energy balances for the riser and down comer [17]. These were merged using a continuity equation applied to the riser and down comer to produce an unambiguous representation for superficial fluid velocity.

$$V_{Lr} = \left[\frac{2gh_D(\epsilon_r - \epsilon_d)}{K_B \left(\frac{A_r}{A_d} \right)^2 \frac{1}{(1 - \epsilon_d)^2}} \right]^{0.5} \quad (41)$$

Equation 41 is a first model. By setting ϵ_d to zero changes in V_{Lr} could be related to changes in ϵ_r . ϵ_r was not an input. Equation 42 related this to an input. It is based on modelling gas hold-up within bubble columns. Hudson [1] suggested liquid-gas up flow within a riser is the same as concurrent gas-liquid flow in bubble columns. So, equations created for them could be applied here and Equation 42 was used for initial modelling [10].

$$\epsilon_r = \frac{V_{Gr}}{0.24 + 1.35(V_{Gr} + V_{Lr})^{0.93}} \quad (42)$$

In addition, equation 42 contains the term V_{Lr} . So, combining the two equations (41 and 42) and reorganising produces an implicit function with V_{Lr} depending on V_{Gr} . Other terms were fixed by reactor geometry. Equation 43 shows the resulting equation; a cubic polynomial. Solving the equation for values of V_{Gr} produces a steady state value for V_{Lr} for each V_{Gr} value.

$$V_{Lr}^3 + V_{Lr}^2(V_{Gr} + 0.177) - \frac{1.148gh_D V_{Gr}}{K_B \left(\frac{A_r}{A_D} \right)^2} = 0 \quad (43)$$

A Newton-Raphson iterative technique was used to solve equation 43. V_{Lr} was initially assumed to be zero for $V_{Gr} = 0$ because there would not be any circulation without any input. V_{Gr} was incremented and for every new value a new V_{Lr} was calculated; the value from the previous calculation formed the estimation for the next. Only the relevant (real) root of the polynomial was used.

5.1. Testing the first model

Calculations were contrasted with those described by Verlaan [22] and calculations were made for a HRAR, but actual data could not be found to check them. Table 2 shows some data used for testing.

The superficial fluid velocity was undervalued by 3.9 for the superficial gas velocity. The shape of the line was similar and that suggested that the form of the model was correct. Hudson [1] used a loss coefficient KB to account for resistance of a valve between down comer and riser in the arrangement they were using [17]. Pipe wall loss was negligible in compared to valve losses and so were they ignored them. The loss coefficient KB was reduced from 4.62 (quoted in [22]). Instead a value of 0.15 was used. The first model then accurately predicted superficial liquid velocity [10].

Some results from testing predictions from the first model for a HRAR are shown in Fig. 7. Superficial gas velocity was adjusted from ICIs estimation and a loss coefficient KB was randomly set to a 4.0. There were not any measured velocities to compare, but results were the correct magnitude.

Figure 6 here. Results for the first model (Test 1 Results)

Results are shown in Fig. 6. There was disagreement between predicted velocities and actual measured velocities.

Table 2 here. Test data from the first model

5.2. Discussion of results concerning the first model

Initial results were of the correct form but only $\frac{1}{4}$ of the values anticipated. An explanation could be that the

loss coefficient value was not correct. The value of 4.62 was initially used from [22,23].

Figure 7 here. More data from testing the first model

Hudson [1] quoted a loss coefficient of:

$$K_B = 11.402 \left(\frac{A_d}{A_b} \right)^{0.789} \quad (54)$$

where: A_b = free area of fluid flow at the base of the “U” tube [10].

Considering the size and proportions used for the reactor in Test 1, and a loss coefficient of 0.15, a close fit was achieved with test data. Equation 44 forecasted an A_b value for the reactor of 2m². That was unrealistic. Using a value of 4.62 the A_b value was 0.0247m² for a connecting pipe diameter of 0.177m; only just too big. That suggested the model in Equation 43 would constantly under-predict the circulation velocities. The shape of the resulting graphs were realistic but superficial liquid velocities were well below those predicted. This was compounded by including down comer void fraction, which slowed the reactor.

Calculations for riser void fraction included a degree of empiricism within the formula as it was based on a bubble column reactor (without any net fluid flow). HRAR is an airlifter so that parameters and possibly calculations were probably different. Hudson [17] suggested liquid-gas flowing up the riser is identical to concurrent fluid-gas flow in a bubble column. So, equations developed for the latter would also be applicable to airlift reactors. But the research only considered small-scale apparatuses and the assumptions may be invalid.

Some factors were neglected by the model. These included: changing void fraction because of pressure change with depth, solubility of gas, and the specific flow regimes that might happen as void fraction changed. Turbulence effects and linear liquid velocity change was not considered. Skin friction loss was noted but disregarded for the time being. Working at a small-scale, these exclusions and exceptions may be tolerable, but in HRAR, pressures and velocities are much bigger. In addition, the size of the reactor means these factors would almost certainly be of significance.

It may have been possible to improve this initial model but the amount of estimation would always restrict its use for HRAR design. Instead, a different model was created to improve the design program.

6. IMPROVING THE DYNAMIC MODEL

The newer model endeavoured to embrace all the parameters that might affect dynamics in the system. The model considered liquid-gas drag forces, flow regimes in the riser and down comer, as well as wall drag (down comer and riser). It was assumed that mass transfer did not occur between gas and liquid, so it was possible to use continuity equations for the fluid in addition to the gas phase. The model was extended from Joshi *et al* [24] as described in [10].

The newer 2nd model balanced driving and resisting forces around a HRAR:

$$\int \rho_L (1 - \varepsilon_d) g dz - \int \rho_L (1 - \varepsilon_r) g dz = \int \left(\frac{d \Delta P_f}{dz} \right) dz \quad (45)$$

Down comer	Riser	Reactor
hydrostatic	hydrostatic	friction
pressure	pressure	pressure loss

Any secondary losses in the head tank and turn at the bottom were neglected. Equations for two-phase flow and void fraction were needed to calculate a balance.

6.1. Flow Regime Identification

Joshi found that a bubbly flow regime prevailed in pipes with a diameter of more than 2/10 m and for superficial velocities found within HRAR [24]. In vertical up flow segments such as a riser, two different flow regimes were suggested: heterogeneous and homogeneous [24,25]. Heterogeneous flows take place at bigger superficial gas velocities of greater than 0.5 ms⁻¹. Internal recirculation of fluid occurs and various sizes of bubbles and varying void fraction profiles are seen. During homogeneous flow, void fraction is unchanging in a radial direction. It takes place at small superficial gas velocities of less than 0.05 ms⁻¹. Transition between regimes depends on influences such as the design of the sparger, size and shape of the column, surface tension, liquid and superficial liquid velocity [24]. In order to detect a transition from one regime to another, a local volumetric flux of gas phase against void fraction was plotted [10,17]. When flux increased suddenly for a small void fraction increase, then that point was identified as a transition. Pressure increased with depth and that decreased void fraction. So any propensity for heterogeneous flow decreased. If the

injected gas did not go above the void fraction at which the flow reversed (critical void fraction) then homogeneous flow prevailed within the down comer [24]. Nichol also observed this during PhD studies [10] and Joshi stated that heterogeneous flow predominated within the riser [26]. That was assumed within the new model.

6.2. Calculations for Void Fraction

Specific experimental data was needed to estimate void fraction, because the behaviour can be sensitive to lots of influences such as sparger design, liquid phase physical properties, column diameter and the phase superficial velocities.

By definition, void fraction was constant within homogeneous flow in the radial direction. It was determined from gas phase mass balance providing bubble rise velocity was known.

Joshi [24] described excellent predictions provided by the Lockett & Kirkpatrick correlation:

$$-\frac{V_G}{\varepsilon_G} + \frac{V_L}{\varepsilon_L} = V_s = (1 - \varepsilon_G)^{1.39} (1 + 2.55 \varepsilon_G^3) \quad (46)$$

The heterogeneous regime had non-uniform void fractions and velocities. A sizeable fraction of gas can within a central part of the flow. So, averaging was required to compute outcomes from the gas phase mass balance. Zuber & Findlay [27] proposed a widely used model that accounted for changes in slip between phases which might occur due to non-uniform flow profiles. Sanders [10], Hudson [17] and Gomezplata [28] developed some similar models. The model described by Zuber & Findlay [27] was adopted:

$$\varepsilon_G = \frac{V_G}{C_0(V_G + V_L) + C_1} \quad (47)$$

where: C_0 = distribution coefficient

C_1 = distribution constant

C_0 and C_1 catered for change in flow along the reactor, based on fluid and superficial gas velocities and void fraction. A distribution coefficient was defined:

$$C_0 = \frac{\varepsilon_G(U_G + U_L)}{\varepsilon_G(V_G + V_L)}$$

If C_o was one then flow was homogeneous. It reduced as C_o increased. C_i was considered constant at first but was eventually defined as:

$$C_i = \frac{\varepsilon_G \varepsilon_L V_s}{\varepsilon_G} \quad (49)$$

The Zuber & Findlay (1965) correlation has been used by many researchers to correlate their void fraction data for different ranges of conditions [17]. Joshi [24] reported analysis of data for reactors with a net fluid flow, and suggested use of an experimental correlation of C_o against superficial liquid velocity [17].

$$C_o = 2 - 1.263V_L + 0.547V_L^2 - 0.073V_L^3 \quad (50)$$

If $C_o < 1.16$, C_o needs to be 1.16. C_i is 0.3 for superficial liquid velocities ranging from zero to 2.4 ms^{-1} .

The Zuber & Findlay [27] correlation was used in both riser and down comer calculations.

6.3. Frictional Pressure Drop

The Darcy formula for single-phase pressure drop within a pipe was used to calculate frictional pressure drop. It was multiplied by Φ_L^2 (a two-phase friction multiplier) to account for extra loss due to phase interaction.

$$\Delta p_f = \frac{2f\rho_L V_L^2 L}{D} \phi_L^2 \quad (51)$$

A model developed by Ranade [29] was used for the two-phase multiplier. It depended on flow regime. For homogeneous flow:

$$\phi_L^2 = \frac{1}{\varepsilon_L^2} + \frac{4.5}{f} \left(\frac{\varepsilon_G V_s}{V_L} \right)^2 \quad (52)$$

The correlation of Joshi [24] was used for heterogeneous flow:

$$\phi_L^2 = \frac{1}{\varepsilon_L^2} + \frac{2 u_{yb}^2}{f V_L^2} \quad (53)$$

where additional turbulence because of bubbles u'_{yb} was determined from:

$$u'_{yb} = 0.25 \left[gD \left(V_G - \frac{\varepsilon_G}{(1 - \varepsilon_G)} V_L - \varepsilon_G V_s \right) \right]^{\frac{1}{3}} \quad (54)$$

The Moody correlation was used to calculate friction coefficient f . It was used to calculate two-phase and single-phase drops in pressure:

$$f = 0.001375 \left[1 + \left(20000 \frac{k}{d} + \frac{10^6}{Re} \right)^{\frac{1}{3}} \right] \quad (55)$$

Reynolds number depended on linear liquid velocity U_L . That was predicted from superficial liquid velocity:

$$U_L = \frac{V_L}{(1 - \varepsilon_G)} \quad (56)$$

Other influences, for example viscosity, density and diameter were presumed constant. This meant that it was possible to calculate the Reynolds number:

$$Re = \frac{\rho_L d U_L}{\mu_v} \quad (57)$$

6.4. Superficial Gas Velocity

An first superficial gas velocity was carefully chosen, V_G . It was needed to give an opening point for integrating forces around the “U” tube. A constant for gas flow around the reactor was molar flow rate G as molar flow rate was unaffected by pressure variations, and as it was presumed that mass transfer did not take place between liquid and gas. Once V_G was at the injection point then volume flow rate was evaluated. Molar flow rate was obtained using the ideal gas equation:

$$G = \frac{P \dot{V}_G}{\tilde{R} T} \quad (58)$$

where: P = pressure at injection point.

Superficial gas velocity varied with pressure while molar flow rate remained the same. That permitted V_G to be determined for any local pressure by using the ideal gas equation in reverse:

$$V_G = \frac{G \tilde{R} T}{A P}$$

7. A SECOND PROGRAM

Solving equations within the 2nd program depended on an iterative process:

1. Estimate superficial gas velocity at air-input.
2. Calculate and sum static and frictional pressures in steps from the top of the down comer to the bottom (steps were 1m apart).
3. Repeat summing procedure for the riser (from the top down to the bottom).
4. Calculate the disparity between static pressures at the bottom of the “U” tube.
5. Calculate total frictional pressure drop within the “U” tube (the riser and the down comer).
6. If the values produced by Step 4 and Step 5 are equal then reactor flow was balanced. If not then the estimate of the superficial gas velocity was changed and Steps 1 to 6 repeated.

7.1. Testing the second program

Initial trials took place to find the effect of changing parameters on the pressure balance around the reactor [30]. A typical HRAR configuration is shown in Table 3.

Table 3 Typical HRAR configuration for testing

Outputs monitored for the tests were: down comer static pressure; riser frictional pressure; down comer frictional pressure and riser static pressure. Total reactor frictional pressure and static pressure difference at the base could then be calculated from them. Tests exhibited larger than expected drops in friction pressure within the riser, typically 10 x static pressure difference. This was being caused by the heterogeneous two phase frictional multiplier. It was delivering multiplication factors > 7500. It would normally only be about 250. The extreme values were because of Equation 44. If V_s was substituted from Equation 40 then Equation 44 becomes identically zero. That was clearly not correct.

$$V_s = \frac{V_G}{\varepsilon_G} - \frac{V_L}{(1 - \varepsilon_G)}$$

To correct this, the model within the second program used the homogeneous friction coefficient for riser calculations as well as for down comer calculations.

Figure. 8 and Fig. 9. show results from varying superficial liquid velocity. Figure 8 shows friction pressure and static pressure drop for both the riser and the down comer. Figure 9 shows the resultant friction pressure and reactor static pressure reduction.

Figure 8 here. Down comer and Riser Pressure Profiles

Figure 9 here. Reactor Pressure Profiles

8. EVALUATION OF THE IMPROVED PROGRAM

The 2nd program forecast reducing frictional loss in the riser for an increase of superficial liquid velocity. No such decrease showed within the down comer, where superficial liquid velocity was the same as in the riser (because cross sectional area was the same). This may have been due to decreasing gas void fraction resulting from increases in superficial liquid velocity. This decreased the homogenous friction multiplier. This merits additional research as single phase frictional loss is proportional to superficial liquid velocity squared [17,31,32].

9. CONCLUSIONS

This paper has described the models used to develop programs to describe two phase pipe flow, including flow pattern identification, two-phase pressure loss and correlations for gas void fractions. A short review of airlift reactor models was also included within the text.

The Clark & Flemmer model was elaborated from analysis. It provided a precise correlation.

Research was supported by EffTech Ltd and they supplied design programs (and their help and knowledge).

HRARs have been designed using a program written by ICI. The basics of wastewater treatment and

the HRAR process within it were examined. The design program (called APRPC-V) was complicated and there was little documentation. A decision was made to write a new structured program to replace APRPC. Because the new program is structured, modules can be replaced as they are improved or new better modules are developed.

The work then moved on to investigate new methods of modelling HRARs. Two models were constructed. The first model within the new program was relatively simple, but it helped to develop an understanding of the requirements for further modelling of a HRAR. The second model was more comprehensive and considered flow regimes in reactor, wall drag & gas/liquid drag forces. That model was used to improve the program. Preliminary testing indicated results of correct order & magnitude.

Future work will focus on creating AI to improve the HRAR design program performance. That new work has begun by investigating expert systems to provide an appreciation of how to structure an expert system using production rules in VB that can easily interface to the new program. Fuzzy logic could be useful for this application as it is good when there is some uncertainty. Preliminary investigations into creating these types of systems for the program are being investigated. An expert system could prove to be more useful though.

To conclude, design of HRARs has been investigated and a new structured design program was created. Modelling of steady state fluid dynamics was then updated to improve the new program.

REFERENCES

- [1] Hudson A. D., "A new blackboard framework applied to a HRAR design program", *PhD Thesis*, Univ. of Portsmouth, 1998.
- [2] Fields P. R., "The ICI Deep Shaft Process", *Meeting of the North East Centre Institute of Wastes Management*, 18 Oct. 1991, ICI Wilton Centre, UK, 1991.
- [3] Merchuk, J. C., Airlift bioreactors: Review of recent advances. *6th International Conference on Gasliquid and Gas-Liquid-Solid Reactor Engineering*, Vancouver, Canada Aug 17-20, 2003. *Canadian Journal of Chemical Engineering Vol: 81 Issue: 3-4, pp: 324-337*. 2003.
- [4] Gray N. F., Activated Sludge. *Biology of Wastewater Treatment: 2nd, pp. 465-639. doi: 10.1142/9781860945243_0005*. 2004.
- [5] Petersen, EE; Margaritis, A. Hydrodynamic and mass transfer characteristics of three-phase gaslift bioreactor systems. *Critical reviews in biotechnology, Volume: 21 Issue: 4 Pages: 233-294*. 2001
- [6] Wang, T.; Wang, J.; Jin, Y., Slurry reactors for gas-to-liquid processes: A review. *Industrial & Engineering Chemistry Research Vol: 46 Issue: 18, pp: 5824-5847*. 2007.
- [7] Ramos, C; Eugenia S-O. Maria; Carrera, J., Long-term performance and stability of a continuous granular airlift reactor treating a high-strength wastewater containing a mixture of aromatic compounds. *Hazardous Materials Vol: 303, pp: 154-161*. 2016.
- [8] Jamshid Behin, Negin Farhadian, Mojtaba Ahmadi, Mehdi ParviziOzone assisted electrocoagulation in a rectangular internal-loop airlift reactor: Application to decolorization of acid dye, *Journal of Water Process Engineering, Volume 8,pp: 171-178*. 2015.
- [9] Talvy, S., Cock, A. and Alain L. "Global modelling of a gas-liquid-solid airlift reactor". *Chemical Engineering Science*,

- [10] Sanders D.A., Cawte, H and Hudson A.D. “Modelling of the fluid dynamic processes in a high-recirculation airlift reactor”. *International Journal of Energy Research*, 25 (6), pp: 487–500, DOI: 10.1002/er.698. May 2001.
- [11] Sanders D.A. and Hudson A.D. “A specific blackboard expert system to simulate and automate the design of high recirculation airlift reactors”. *Mathematics and Computers in Simulation*, Vol 53 (1–2), pp: 41–65. Aug 2000.
- [12] Sanders D.A., Hudson A.D, Tewkesbury G.E. and Mason S. Automating the design of high-recirculation airlift reactors using a blackboard framework. *Expert Systems with Applications*, Volume 18, Issue 3, pp: 231–245. April 2000.
- [13] Danckwerts P. V., “Gas Liquid Reactions”, McGraw Hill, 1970.
- [14] ICI, “Deep Shaft Effluent Treatment Process”, Book 2, *Engineering*, 1991.
- [15] Verlaan P., Jan-Chris, V. and Riet K. C. T. “Axial dispersion and oxygen transfer in the transition from bubble column to airlift-loop reactor”. *Jrnl Chemical Technology and Biotechnology*, Vol 45 (3), pp: 181–190. Apr 2007.
- [16] Zhao, J., Xie, J., Lin, H., and Hu, W. “Experimental study on two-phase gas-liquid flow patterns at normal and reduced gravity conditions”. *Science in China Series E: Technological Sciences*, Vol 44 (5), pp 553-560. 2001.
- [17] Hudson A. D., “General blackboard framework for high recirculation airlift reactors”, PhD Thesis, Univ. of Portsmouth, 1997.
- [18] Soare, A Pérez Escobar S. A., Stankiewicz, A. I., Pascual, M, R and. Kramer H. J. M. “2-D Flow and Temperature Measurements in a Multiphase Airlift Crystallizer”. *Ind. Eng. Chem. Res.*, 52 (34), pp 12212–12222. 2013.
- [19] Coulson J. M. and Richardson J. F., “*Chemical Engineering*”, Vol. 1, Pergamon, 1970.
- [20] Guettel, R and Turek T, “Comparison of different reactor types for low temperature Fischer–Tropsch synthesis: A simulation study”. *Chemical Engineering Science*, Volume 64, Issue 5, pp: 955–964. Mar 2009.
- [21] Klein J., Godo, S., Dolgoš, O. and Markoš, J. “Effect of a gas–liquid separator on the hydrodynamics and circulation flow regimes in internal-loop airlift reactors. *Jrnl of Chemical Tech and Biotech*, Vol 76 (5), pp: 516–524, May 2001
- [22] Verlaan P., Vos J.-C. and van’t Riet K., “Hydrodynamics of the Flow Transition from a Bubble Column to an Airlift-Loop Reactor”, *Jnl. Chem. Tech. Biotechnol.*, Vol. 45, No 2, pp 109 - 121, 1989.
- [23] Verlaan P., Tramper J., van’ Riet K. and Luyben K., “A Hydrodynamic Model for an Airlift-Loop Bioreactor with External Loop”, *Chem. Eng. Jnl.*, Vol. 33, pp B43 – B53, 1986.
- [24] Joshi J. B., Ranade V. V., Gharat S. D. and Lele S. S., “Sparged Loop Reactors”, *Canadian Jnl. Chem. Eng.*, Vol. 68, No 5, pp 705 – 741, 1990.
- [25] Shah Y. T., Kelkar B. G., Godbole S. P. and Deckwer W.-D., “Design Parameters Estimation for Bubble Column Reactors”, *AIChE Jnl.*, Vol. 28, pp 352 – 379, 1982.
- [26] Joshi J. B., “Hydrodynamic and Mixing Model for Bubble Column Reactors”, *Chem. Eng. Commun.*, Vol. 11, pp 165–199, 1981.
- [27] Zuber N. and Findlay J. A., “Average Volumetric Concentration in Two-Phase Flow Systems”, *Jnl. Heat Transfer*, Vol. 87, pp 453 – 468, 1965.
- [28] Gomezplata A., Munson R. E. and Price J. D., “Correlation of Two Phase Void Fraction Data”, *Can. Jnl. Chem. Eng.*, Vol. 50, pp 669 – 671, 1972.
- [29] Ranade V. V., Gharat S. D. and Joshi J. B., “Pressure Drop in Multiphase Reactors”, *Recent Trends in Chem. Reaction. Eng.*, Wiley Eastern Publ., New Delhi, pp 164 – 180. 1987.
- [30] Hudson AD, Sanders AD, Tewkesbury GE, Cawte H and Hinks J., “Simulation of a high recirculation airlift reactor for steady state operation”, *Wat Sci Tech*, Vol 34, No 5-6, pp 59 - 66, 1996.
- [31] Hudson AD, Sanders AD, Golding H, Tewkesbury GE and Cawte H., “Aspects of an expert design system for the wastewater treatment industry” *Journal of systems architecture* 43 (1997) pp 59 – 65, 1997.
- [32] Hinks JW, Cawte H, Sanders DA, Hudson AD, and Dockree CN., “Prediction of flow rates and stability in large scale airlift reactors”, *Wat Sci Tech*, Vol 34, No 5-6, pp 51-57, 1996.