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    -OF CONTENT, OMISSIONS: EDITING YOUR DRAFT IS VERY HARD.
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- YOU CONFUSE AN UNDERGRADUATE REPORT WITH A

GRADUATE THESIS.

- YOU CONFUSE A TANK WITH A REACTOR
- AT LEAST 50% OF THE DRAWINGS SHOULD BE YOURS <u>NOT</u> FROM CUT AND PASTE REFERENCES (SEE SECTION 2).
- EACH VARIABLE MUST INCLUDE THE UNITS IN (BRACKETS).
- YOU CUT AND PASTE EQUATIONS WITHOUT EXPLAINING THEIR MEANINGS.
- YOUR INTRODUCTION IS VERY SHORT AND HAS NO CONTENT.
- STUDY <u>ALL</u> THE PUBLICATIONS BY REZA AND ALVAREZ CUENCA. THEY ARE THE BEST SOURCE OF INFO.
- CHECK YOUR SPELLING AND GRAMMAR. YOU HAVE TOO MANY MISTAKES.
- PARTS OF THE TEXT APPEAR TO HAVE BEEN WRITTEN BY A
  - NON-NATIVE ENGLISH SPEAKER.

- DON'T USE THE WORD <u>SYSTEM</u> FOR ANYTHING THAT YOU CANNOT EXPRESS.
- EXPLAIN PROPERTIES AND APPLICATIONS OF GAMMA FUNCTION IN THE APPENDIX.
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- SOME FIGURES (2.1, 2.6) DO NOT HAVE ANY COMMENTS IN THE TEXT, THIS MAKES MEANINGLESS THE READING OF THE DRAFT.
- HOW CAN YOU HAVE 69 REFERENCES AND SUCH A BRIEF

## INVESTIGATION OF THE FLOW DYNAMICS OF A VERTICAL BIOREACTOR USING THE RESIDENCE TIME DISTRIBUTION

by

### Mark Edney

BEng Ryerson University 2011

A thesis presented by Ryerson University

In partial fulfillment of the

requirements for the degree of

Master of Applied Science

in the program of

Chemical Engineering

Ryerson University

Toronto, Ontario, Canada, 2020

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August 6, 2020

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Investigation of the flow dynamics of a Vertical Bioreactor using the Residence Time Distribution

Mark Edney, Master of Applied Science, Chemical Engineering 2020 Ryerson University

### **Abstract**

In the wastewater industry, conventional activated sludge processes are still the dominant technology.

This technology relies on large concrete tanks with poor mixing profiles and high excavation and materials costs.

In this study, the mixing and fluid flow through the reactor is investigated using residence time distribution tests. We introduced A single pulse of conductive tracer was injected into the first stage of the reactor. Conductivity sensors were used to measure tracer concentration at the exit of each stage. This conductive tracer represents an introduced element through the process flow. Data generated from this experiment found evidence of a bypass rate of 7.5% of the feed rate. The data were compared with two theoretical models: The Ideal Continuous Stirred Tank Reactor and the Generalized Nth CSTR in series model and were found to approximate the curve of the residence time distribution.

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### Acknowledgments

I would like to thank my co-advisors Dr. Maryam Reza and Dr. Samant Upreti for their expert knowledge, which has been instrumental for this research. I give my sincerest appreciations to my advisor Dr. Manual Alvarez Cuenca for both providing me the opportunity and the challenge to grow as a researcher. All of my work would be impossible without the generosity and the facilities of the Chemical Engineering Department at Ryerson University.

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List of Appendices

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### : Introduction

### CHAPTER NUMBER?

The vertical bioreactor has been shown to be a novel reactor for Biological Nutrient Removal (BNR) in water engineering. It has an effective nitrogen-compounds removal rate of 95% and an effective phosphorus removal-rate of 90%[1]. It has been proposed to have superior mixing and mass transfer due to its tubular geometry[2].

A model <u>has not been created</u> to simulate the flow dynamics of the vertical bioreactor. As outlined by Levenspiel, modelling a chemical reactor requires three parts[3]:

- The Residence Time Distribution
- A Model
- Reaction kinetics

The purpose of this experiment is to determine the mixing profile exhibited by the vertical bioreactor. This mixing profile will be used to examine different reactor models, finding a model that will fit the true behaviour of the reactor. This was achieved by introducing a traceable element in the reactor and monitoring the concentration change as it exits each stage of the multi-stage reactor. Collecting this concentration data has enabled the development of the mixing profile or the residence time distribution. The different flow characteristics can be obtained from the collected data.

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### **CHAPTER NUMBER?**

### Literature Review

## READ CAREFULLY THE LATEST PUBLICATION BY ALVAREZ CUENCA AND REZA IN THE CANADIAN JOURNAL, AND THEN REWRITE THIS CHAPTER.

### 2.1 Wastewater Bioreactors

In water engineering, no technology that fits every situation. There will always be a trade-off between nutrient removal efficiencies, system complexity and costs. As a result, there is many investigations into different avenues of treatment. The most promising technologies includes Algae-based technologies, Sequencing Batch Biofilm Reactors, Moving Bed Biofilm Reactors and Membrane Bioreactors. The criteria for examining a bioreactor include simplicity, expense, scale, and nutrient removal efficiencies.

### 2.1.1 Algae-based technologies

The application of algae cultures for wastewater treatment has become a developed technology ([4], [5]) but it has not been applied at the piolet pilot and full-scale. The mechanism of phosphorous removal by algae is illustrated in Figure 2.1. Algae cells reach a saturated stage of phosphorous uptake at about 3% phosphorous by dry weight with a critical minimal level of 1%[6]. Algal treatment can take place in a variety of techniques as a suspended solution or as a biofilm. A system using a microporous tissue for cell immobilization has been shown to remove removal 90% of phosphorous and 69-78% nitrogen[5]. Algal growth can even be incorporated in Membrane Bioreactors (MBR) for increased effluent efficiencies(92% nitrogen and 91% phosphorous removal)[7].

There are some disadvantages to this technology. Algae growth is highly dependent on temperature and exposure to light. These demands are particularly difficult for locations at higher latitudes. Since Algae-based systems is still a technology in its infancy, there lacks research on long term studies and at different flow regimes[8].

Acid soluble PolyP Protein & Cell wall

Acid insoluble PolyP Intracellular PO<sub>4</sub><sup>3-</sup>

Lipid & RNA P

FIGURE 0.1: MECHANISM OF ALGAL PHOSPHOROUS REMOVAL[4]

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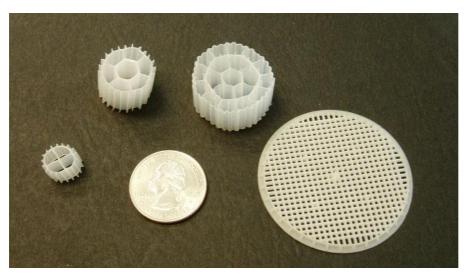


FIGURE 0.2: SAMPLE MEDIA[9]

### 2.1.2 Moving Bed Biofilm Reactors

A Moving Bed Biofilm Reactor (MBBR) functions and operates very similarly to a Conventional Activated Sludge (CAS) process. MBBR include a biofilm that grows on a small suspended carrier (Figure 2.2) that is in constant motion throughout the reactor volume. The media retain microbial populations which aides in the growth of slower developing organisms such as nitrifying bacteria. It is a cost effective and easy way to upgrade CAS reactors. MBBR have been shown to have an effect removal state of 75-97% BOD and 40-85% total nitrogen[9].

In a MBBR, there is a constant collision of media within the reactor. This shearing prevents the development of biofilm on the media outer surface area making the internal surface area of the media an important design factor[9]. Younge has researched the effect of different carrier types and found many noteworthy discoveries[10].

- The highest surface area to volume carriers exhibit the highest level of clogging
- Cellular activity rates of Ammonia Oxidizing Bacteria (AOB) were not affected by carrier type
- Reactor performance is best described by the viable AOB cell coverage of the carriers

The prominent media material is plastic but they provide a low denitrification capacity in MBBR. Research shows that sponge is suitable alternative were it has increased nitrogen removal from 72-86% and phosphorous removal from 70-85%[11]. Also from that study, the sponge material showed less pore blocking and cake layer resistances.

One of the disadvantages of a MBBR is the lack of research in mechanism of biofilm detachment. It is a complicated function of hydrodynamics, flow velocity, biofilm morphology and support characteristics[9]. An additional liquid-solid separation unit to recover media and return them to the reactor entrance.

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### 2.1.3 Sequencing Batch Biofilm Reactors

A Sequencing Batch Biofilm Reactor (SBBR) is a modification of the traditional Sequencing Batch

Reactors (SBR). It includes a media material which aides in the development of attached microbial growth as with a Moving Bed Biofilm Reactor. They seek to combine the advantages of an activated sludge process with a biofilm process. SBBR has been shown to be more efficient than the activated sludge SBR but at the cost of an increase in the process knowledge requirement[12]. Figure 2.3 outlines the schematic of a SBBR.

The activated sludge and the attached growth cultures in a SBBR are identical but at different proportions[13]. Anaerobic Ammonium Oxidation (ANAMMOX) bacteria, bacteria than can reduce ammonium directly to nitrogen gas, are found in higher concentrations in the attached growth[13]. SBBR can achieve high levels of total nitrogen and total phosphorous removal (94% and 97%) as they can provide an environment for Phosphate Accumulating Organisms (PAO), denitrifying phosphate accumulating organisms (DPAO), nitrifying and denitrifying bacteria without carbon source competition[14].

There are some several drawbacks as SBBR are prone to clogging[15]. There is also the potential of floating or settled sludge in the effluent as there is no clarifier unit in the design[16].

Recycle for total N removal

Fill

About 70-98% of the ammonium is used for biomass growth

Aeration About 70-98% of the ammonium is oxidized to nitrite than nitrate

Reduction of oxidized compounds (nitrite and nitrate) to gaseous dinitrogen by heterotrophic bacteria

FIGURE 0.3: SEQUENCING BATCH BIOFILM REACTOR SCHEMATIC[12]

### 2.1.4 Membrane Bioreactors

Membrane bioreactors (MBR) are likely the most popular bioreactors that has attracted a large amount of research. MBRs are recognized as the replacement of the secondary clarifier of the conventional activated

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sludge process with membrane filtration[17]. MBRs are an attractive option for retrofitting conventional plants due to its small footprint and high quality effluent [18].

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One of the main advantages of the MBR over Conventional Activated Sludge (CAS) process is a higher concentration of slowly growing microbes[19]. This is particularly as nitrifying bacteria exhibit this behaviour. Disadvantages

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The best phosphorous removal performance comes from incorporating MBR in hybrid configurations. Membranes utilized well established Biological Nutrient Removal systems, such as the University of Cape Town, have been shown to have phosphorous removal rates of 88%[20] and 87%[21]. Without this additional consideration, the phosphorous removal for MBR can be quite low at 53%[22]. Bracklow preformed a series of four different recirculation schemes with different arrangements of three stage reactors (anaerobic\anoxic\aerobic) and found that there was insignificant differences in nutrient removal rates between schemes. The average removal rates were 97% COD, 88% nitrogen and 99% phosphorous[23].

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Membrane aerated biofilm reactors (MABR) are more complicated systems than MBR. Rather than using the membrane for separation, pressurized air on one side of the membrane while water flows co-current on the other side (Figure 2.4). A biofilm than develops on the surface of the membrane. There are significant increase in aeration rates with a MABR when compared to bubble aeration all in a smaller tank size[24]. Through careful control of the dissolved oxygen levels, both nitrifying and denitrifying kinetics can take place in a single stage[25]. MABR have also been shown to have a significant power reduction of up to 86% when compared to CAS mainly due to the efficiencies for aeration[26]. Explain the figure below.

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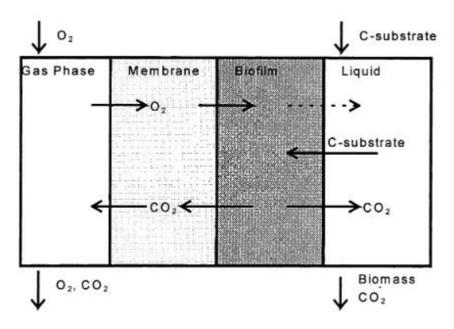


FIGURE 0.4: MEMBRANE AERATED BIOFILM REACTOR[8]

The main difficulty with membranes are their high costs. Their expense comes from two sources, a high initial cost of the modules (50 US%/m² as of 2005[27]) and high maintenance costs. The high maintenance cost comes from the energy demand to deal with membrane fouling. Even after a decade of research and extensive reviews([28]–[30]), there is no consensus on membrane fouling. A lack of standardized fouling characterization method has led to results that sometimes conflict.

### 2.2 Biological Nutrient Removal

### This is a process not a reactor. LEARN THE DIFFERENCE

Biological Nutrient Removal (BNR) is has become an increasingly important field of research. Regulations regarding the concentrations of nutrients in the wastewater industry has become more stringent with chemical or biological treatments available. Biological treatments are the more economical and effective solution Compare to what?[31].

The two components of nutrients in wastewater are nitrogen and phosphorous Negligent treatment (???) can lead to eutrophication. Eutrophication is caused by the over stimulation of algae growth due to the higher concentrations of nutrients. Excessive algae growth increases the rate of algae death (what does this mean????). The necessary bacteria for the decomposition of this increased algae death are incapable of keeping up. This creates layers of decaying material on the bottom of the body of water. The body of water has changed to a green colour and the decaying has started to produce an edour. This darkening of the water, decreases that mass transfer of oxygen into the water. The initial wildlife response can be deceptive with increased fish populations from the increased food source. The

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increased in microbial activity and the decrease in mass transfer reduces the concentration of dissolved oxygen. Fish can no longer obtain the oxygen they require for respiration, increasing the amount of decaying material.

Phosphorous and nitrogen play two different roles in microbiological life and ass such require two distinct sets of reaction kinetics.

### 2.2.1 Biological Nitrogen Removal

Traditional nitrogen removal has been treated as a three-stage process: Hydrolysis and Ammonification, Nitrification and Denitrification (Figure 2.5). The first two processes take place under aerobic conditions (presence of dissolved oxygen) while the Denitrification step takes place under anoxic conditions (no dissolved oxygen but the presence of other dissolved oxygen compounds). Hydrolysis and Ammonification is the process for the conversion of particulate organic nitrogen into soluble ammonia. Ammonia is then oxidized by nitrosomonas and nitrobacter bacteria into nitrites and nitrates respectively. Heterotrophic bacteria can than reduce nitrates into nitrogen gas[32].

This is a simplified model of the biological nitrogen removal process that does not well represent current developments in the field([33], [34]) but it should be sufficient for the understanding of the operating conditions and principles of BNR processes.

Aerobic Conditions

Organic Hydrolysis Ammonia Nitrification Nitrite/ Nitrogen Gas

FIGURE 0.5: BIOLOGICAL NITROGEN REMOVAL FLOW CHART

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FIGURE 0.6: SKELETAL STRUCTURE OF ATP

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### 2.2.2 Biological Phosphorous Removal

The main biological role of phosphorous is facilitating the storage of energy. Cells including microbes use a compound called Adenosine Triphosphate (ATP). The <u>skeletal structure can be found in Figure 2.5</u>. The phosphorous bonds require a large amount of energy to form and likewise releases a lot when broken. When ATP under goes hydrolysis into Adenosine Diphosphate (ADP), the reaction releases 7.4kcal/mole.[35] ADP still has two more phosphorous bonds, which can further hydrolyze releasing more energy.

All heterotrophic bacteria in the activated sludge utilize phosphorous but at relatively low concentrations (0.02 mgP/mgVSS) with a removal rate about 15-25%. Additional phosphorous removal requires selecting for Phosphorous Accumulating Organisms (PAOs). PAOs have a higher utilization rate of phosphorous (0.38mgP/mgVSS) but evolutionary speaking they are non-competitive[36]. In the wild frenzy of the activated sludge microbiome, storing energy is not a good strategy. Microbes that utilize energy to grow or to divide will quickly outnumber microbes that store energy. It is because of this non-competitive nature of PAOs that operating conditions must be optimized for their selection.

In the anaerobic stage (Figure 2.7), PAOs uptake volatile fatty acids (VFA) to create long carbon chains called polyhyrdoyalkanoates (PHA). The cells use their internal energy by breaking Phosphorous

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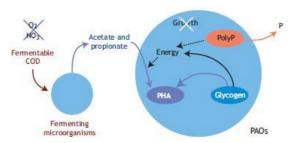


FIGURE 0.7 BIOCHEMICAL MODEL FOR PAOS UNDER ANAEROBIC CONDITIONS [10]

bonds which releases phosphorous in the wastewater. Thus the PAOs absorb VFA which other heterotrophic bacteria are incapable to[36].

In the aerobic stage (Figure 2.8), PAOs digest the newly formed PHA with the dissolved oxygen playing the role of a electron acceptor. This digestion releases energy for the cell, which it can use for cell growth. The excess energy is stored in the form of poly-phosphates (such as ADP and ATP) which facilitates phosphorous transfer from the wastewater into the cell. Phosphorous is than fully removed from the BNR reactor as it is trapped in wasted sludge[36].

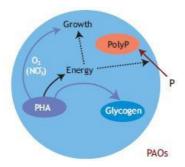


FIGURE 0.8: BIOCHEMICAL MODEL FOR PAOS UNDER AEROBIC CONDITIONS[10]

<u>Traditional</u> it has been suggested that organism in the Acinetobacter group as the ideal PAO population[37]. Nguyen has found <u>that</u> Tetrasphaera bacteria in many different Enhanced Biological Phosphorous Removal (EBPR) plants in higher levels than Acinetobacter. This is of interest as Tetrasphaera exhibit a more flexible substrate uptake[38]. Through a gene study, it was confirmed that Tetrasphaera is capable of denitrification[39]. These are important developments as they can change the model of EBPR and <u>effect</u> the design of Biological Nutrient Removal (BNR) treatment plants in the future.

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### 2.2.3 Activated Sludge Models

The chemical reaction kinetics of wastewater treatment processes have been a field of study for many years and the most influential model is the Activated Sludge Model (ASM). The initial ASM model was limited as it only pertained to the removal of the carbon components. It did however introduce the matrix model, which simplifies the expression of the series of different chemical reactions taking place. The reaction kinetic table can be found in Figure 2.9[40]. This is a significant development as it organizes the reactions where each column represents the mass balance for a component and each row represents a specific chemical reaction. Organization is required as more development into the field increases the number of reactions and number of substrates.

The different reactions are based on the Monod equation, which is defined as:

$$\mu = \mu_{max} \frac{S}{K_S + S} \tag{2.1}$$

Where  $\mu$  is the growth rate,  $\mu_{max}$  is the max growth rate, S is the substrate concentration and K<sub>S</sub> is the half-velocity constant **DEFINE AND INCLUDE THE UNITS OF EACH VARIABLE. Example (mg/L) for concentration.** 

## THE FONTS OF THE TABLE BELOW ARE IMPOSSIBLE TO READ. CHANGE THEM AND MAKE THEM READABLE.

The development in activated sludge models required the addition of nitrogen and phosphorus removal kinetics which were included in the ASM2D model[41]. An increased level of complexity accompanies additional reaction kinetics. As an example, the Activated Sludge Model for

-	Component i	1 Se	2 Xe	3 Хв.н	XB.A	5 Xe	6 Sp	7 S <sub>NO</sub>	8 SNH	9 XND	10 SALK	Process Rate, $\rho_{j}$ , ML- $3\tau^{-1}$
1	Process			0,111		-	-			200	300000	
1	Aerobic growth of heterotrophs	$-\tfrac{1}{Y_H}$		1			$-\frac{1-Y_H}{Y_H}$		-i <sub>XB</sub>		-1 xB	$\Omega_H \left( \frac{S_S}{K_S * S_S} \right) \left( \frac{S_O}{K_O * H * S_O} \right) \times_{B_* H}$
	Anoxic growth of heterotrophs	$-\frac{1}{Y_H}$		1				- 1-Y <sub>H</sub> 2.86Y <sub>H</sub>	-i <sub>XB</sub>		1-Y <sub>H</sub> 14·2.86Y <sub>H</sub> -i <sub>XB</sub> /14	$\mathbb{G}_{\underline{H}}\bigg(\frac{\mathbb{S}_{\underline{S}}}{K_{\underline{S}}*S_{\underline{S}}}\bigg)\bigg(\frac{K_{\underline{O},\underline{H}}*S_{\underline{O}}}{K_{\underline{O},\underline{H}}*S_{\underline{O}}}\bigg)\bigg(\frac{\mathbb{S}_{\underline{N}\underline{O}}}{K_{\underline{N}\underline{O}}*S_{\underline{N}\underline{O}}}\bigg)^{-\eta,\underline{X}}\mathbb{B}_{*}\underline{H}$
3	Aerobic growth of autotrophs				1		- 4.57-YA	$\frac{1}{Y_A}$	$-i_{XB} - \frac{1}{Y_A}$		$-\frac{1}{14}$ $-\frac{1}{71}$	$\mathfrak{g}_{\mathtt{A}}\Big(\!\frac{\mathbb{S}_{\mathtt{NH}}}{\langle \mathbb{K}_{\mathtt{NH}^{+}}\mathbb{S}_{\mathtt{NH}}\rangle}\!\Big)\!\Big(\!\frac{\mathbb{S}_{\mathtt{O}}}{\langle \mathbb{K}_{\mathtt{O}},\mathtt{A}^{+}\mathbb{S}_{\mathtt{O}}\rangle}\Big) \times_{\mathtt{B},\mathtt{A}}$
	"Decay" of heterotrophs		1-f	-1		f <sub>E</sub>				i <sub>XB</sub> -f <sub>E</sub> i <sub>XE</sub>		p <sup>H</sup> X <sup>8</sup> *H
5	"Decay" of autotrophs		1-f <sub>E</sub>		-1	r <sub>E</sub>				i <sub>XB</sub> -r <sub>E</sub> i <sub>XE</sub>		DAXB.A
6	"Hydrolysis" of entrapped organics	1	-1									$ k_{h} \frac{\chi_{q}/\chi_{B_{1}H}}{K\chi^{*}(\chi_{S}/\chi_{B_{1}H})} \bigg[ \bigg( \frac{S_{\square}}{K_{O_{+}H} * S_{O}} \bigg)^{sr_{1}} \bigg( \frac{K_{\square,H}}{K_{O_{+}H} * S_{O}} \bigg) \bigg( \frac{S_{N\square}}{K_{NO} * S_{NO}} \bigg) \bigg] \chi_{B_{1}H} $
7	"Hydrolysis" of entrapped organic nitrogen								1	-1	114	ρ <sub>6</sub> (X <sub>ND</sub> /X <sub>S</sub> )
OR	Observed Conversion			ri - I	vijej							
P He Au Er o Ma	coichiometric arameters: terotrophic yield: Y <sub>M</sub> utotrophic yield: Y <sub>A</sub> ndogenous fraction of blomass: f <sub>E</sub> ass N/Mass COD in clomass: i <sub>XB</sub> ass N/Mass COD in endogenous blomass: i <sub>XE</sub>	Readily biodegradable substrate - M(COD)L-3	Slowly biodegradable substrate - M(COD)L-3	Active heterotrophic biomass - M(COD)L-3	Active autotrophic blomass - M(COD)L-3	Endogenous mass arising from biomass decay M(ODD)L-3	Oxygen (negative COD) M(-COD)L-3	Nitrate and nitrite nitrogen = $M(N)L^{-3}$	NH4 + NH3 nitrogen - M(N)L-3	Biodegradable organic nitrogen = $M(N)L^{-3}$	Bloarbonate alkalinity - Molar units	Kinetic Parameters:  Heterotrophic growth and decay:  \$\begin{align*} \begin{align*} alig

Figure 0.9: ASM 1 Model Table[11]

Nitrogen (ASMN) models 3 different groups of microbes, 18 biological processes, 20 components and contains 54 parameters in total [33].

Commented [WU46]: EXPLAIN THE RELEVANCE AND USEFULNESS OF THIS MODEL

### 2.3 The Residence Time Distribution

## Commented [WU47]: THIS SECTION YOU MADE IT ALL CUT AND PASTE. FIGURES, EQUATION, ALL. CAN YOU MAKE SOME CONTRIBUTION OF YOUR OWN?

### 2.3.1 Definition

Continuous flow systems are categorized into two simplified models, the Plug Flow Reactor (PFR) and the Continuous Stirred Tank Reactor (CSTR). The CSTR model requires the assumption of perfect mixing throughout the reactor while the PFR model requires the assumption that fluid flow into the reactor travels in parallel paths and leave at the same moment. In reality, most systems flows do not well represent either of these cases very well. The assumptions are made however to significantly reduce the complexity of a system. Danckwerts[42] and Zweitering[43] developed a technique to better understand the behavior of a flow system with the Residence Time Distribution (RTD). This incredible development enabled the modeling of continuous systems without the assumptions required for the CSTR and PFR models.

The technique requires the introduction of a traceable element into the continuous flow system.

The traceable element is then measured as it exits the system with a sensor that is specific to the parameter that the element is traceable by. For more information on the process of tracer selection please refer Section 3.1.1 Tracer Selection (pg 35) to A C-diagram can then be created by plotting the concentration of the tracer at the exit versus time. The Population Density Function (E(t)) can then be obtained from dividing the concentration of the tracer by the area under the C-diagram. The area under the C-diagram (or the integral) represents that mass of the tracer injected into the system[44]. The E(t) function represents the probability of the tracer exiting the system at time t when excited by a pulse.

The second RTD function is the Distribution Function (F(t)). The F(t) function represents the fraction of tracer that has exited the reactor at any time. It represents the cumulative sum of the **E(t)** and thus can be represented by the following equation. It also represents the system response to a step change (????).

$$E(t)_{cstr} = \frac{1}{\tau} e^{-t/\tau}$$

$$F(t) = \int_0^t E(t) dt$$
 (2.2)

There are few advantages for using the F(t) rather than the E(t). The E(t) is easier to spot trends and different flow characteristics.

Commented [WU48]: " .....they leave the reactor at the same moment"

Commented [WU49]: Do you have any other word than "System"

Commented [WU50]:

Commented [WU51]: WHAT IS INCREDIBLE ???????

**Commented [WU52]: reactor**. System is a word that means nothing

Commented [WU53]: DID YOU DEFINE WHAT E(t) is?????

Commented [WU54]: Did you show what a step change is?

Commented [WU55]: Rewrite this SECTION

### 2.3.2 Application of RTD Measurements

### The main application for RTD measurements as outlined by Missen are the following [45]:

- 1. As a diagnostic tool for the detecting and characterizing flow behavior
- 2. The estimation of values of parameters for non-ideal flow models
- 3. The assessment of performance of a vessel as a reactor

The graphs that represent the RTD functions for a reactor can be an important tool in identifying issues with the mixing. One such example was when Goswami found the RTD for a constructed wetland described a dead-space in the reactor to be between 0% and 41% [46]. The theoretical residence time, measured by the volume of the reactor divided by the fluid volumetric flow rate, was found to be larger than the experimentally observed mean residence time. This suggests that the tracer did not travel throughout the entire volume. The volume of which the tracer did not travel through is referred as the dead-space because no reaction would take place there.

The simplest application is comparing the reactors RTD to that of the ideal graphs represented in Figure 2.15 & Figure 0.17. It can provide as quick and simple visualization of the discrepancy from the ideal conditions.

The true value of the RTD experiment comes from the creation of the parameters for the non-ideal flow models. Non-ideal flow models seek to represent the flow of real reactors. These models are because every flow model has a unique RTD but not every RTD has a unique flow model. "Real reactor" models are the generated and their RTD calculated. These models are than compared to the experimentally collected results. If the RTD that describes the non-ideal model also fits the experimental data then the non-ideal model also fits flow dynamics of the reactor.

The final application of the RTD is the assessment of the reactors performance. This assessment relies on three factors; whether the fluid behaves as a segregated or a maximum mixedness fluid, when mixing occurs and the reaction order. For a first order reaction, such as  $r_a = kC_a$ , only the RTD effects the conversion as the reaction takes place with a single molecule and doesn't require any sort of collision. For reactions of any other order, the RTD data is not enough[43].

A segregated fluid enters as **globulars** with perfect mixing within each globular but no mixing between them. This is also referred to as a macro-fluid. A micro-fluid, or a **maximum mixedness** fluid, has the opposite behaviour where each element is free to mix fully throughout the system (Figure 2.10). **YOU DON'T EXPLAIN ANYTHING IN TABLE 1. JUST CUT AND PASTE.** 

Commented [WU56]: THE MAIN APPLICATION....." is singular and "are" is plural.

Commented [WU57]: are important tools in

Commented [WU58]: WRITE THEM IN POINT FORM.

Commented [WU59]: And the reaction order what??????

Commented [WU60]: DATA IS PLURAL. DATA "ARE"

Commented [WU61]: Globular is an adjective. Globules is a name.

Commented [WU62]: You mean "perfectly mixed fluid""?

Reaction Order	Conversion
n < 0	$X_{seg} > X_{mm}$
0 < n < 1	$X_{seg} < X_{mm}$
n = 1	$X_{seg} = X_{mm}$
n > 1	$X_{seg} > X_{mm}$

TABLE 1: MICRO-MIXING EFFECT ON CONVERSION BY REACTION ORDER[3]

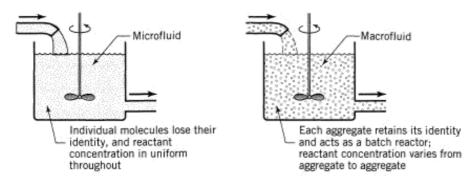


FIGURE 0.10: MICRO VS MACRO MIXING[18]

The relationship between the model of micro-mixing and the reaction order can be complicated but the effects are outlined in Table 1 [47]. It is also important to note that wastewater treatment reactions are often of mixed order, between first and zero[48]. There is no effect on the conversion in a PFR due to the degree of segregation as a PFR can be considered as a flow of batch reactors with the same residence time.

The effect of when the mixing happens was first explored by Zwietering[43]. The simplest way to explain it is illustrating a CSTR and a PFR in series (*Figure 0.11*). No matter the order of the reactors, the overall RTD will be the same. Both systems will have the same overall mixing profile. The second case, where the CSTR proceeds the PFR, mixes much sooner than the alternative.

In reactors with a single reaction, the effects of segregation and earlines of mixing can usually be ignored. For reactors with multiple reactions, such as the vertical bioreactor for the treatment of wastewater, these effects can become more prominent. ...

Commented [WU63]: THE EXPLANATION IS POOR.

Commented [WU64]: ???????

Commented [WU65]: AGAIN YOU CONFUSE REACTORS WITH REACTIONS.

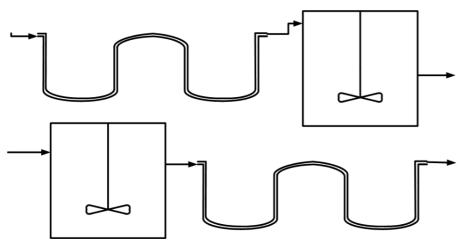


Figure 0.11: PFR than CSTR vs CSTR than PFR

This is a very crude diagram that fails to explain anything.

### 2.3.3 Dead-space and By-passing

Dead-space and By-passing are two undesirable conditions in a reactor as they represent deviations in the Mean Residence Time (MRT). Dead-space is an area within a reactor, which is not utilized for the reaction, it is a zone of stagnation. By-passing refers to the formation of channels through the reactor were reagents do not mix and are not utilized for the reactor. Both represent inefficiencies in

the mixing profile.

These conditions are understood by modeling them[47]. For the definition of the theoretical MRT:

$$\tau = V/v$$

<u>τ is not theoretical is average or mean residence time</u>

WHERE,

V is .....

au is ......

v is ... ...

Your draft needs a great deal of editing

Commented [WU66]: What is this ?MAKE YOUR OWN DRAWING.

Commented [WU67]: THE TITTLE OF THIS FIGURE IS INCOHERENT. WHO DREW THE GRAPH???????

Commented [WU68]: This is What?

**Commented [WU69]:** Mark; YOU HAD NO TIME TO EDIT YOUR DRAFT????????

Commented [WU70]: Dead zones are stagnant but they have undesirable reactions.

Commented [WU71]: MEAN RESIDENCE TIME.

For a system with by-passing, part of the fluid flow doesn't enter the system. The overall flow rate  $(v_0)$  is the summation of the flow that enters  $(v_E)$  and the flow that by-passes  $(v_B)$ :

Commented [WU72]: REWRITE THE SENTENCE

$$v_0 = v_E + v_B$$

Where the observed  $au_{obs}$  MRT is:

$$\tau_{obs} = \frac{V}{v_E}$$
 
$$\tau_{obs} = \frac{V}{v_0 - v_B}$$

And then comparing the ratio of the two MRTs:

$$\frac{\tau_{obs}}{\tau} = \frac{V/(v_0 - v_B)}{V/(v_0)}$$

$$\frac{\tau_{obs}}{\tau} = \frac{v_0}{v_0 - v_B} > 1$$

$$\boldsymbol{\tau_{obs}} = \boldsymbol{\tau} \times (\frac{v_0}{v_0 - v_R})$$

From the last line, it is apparent that for a system with by-passing will have an observed MRT higher than the theoretical  $au_{ullet}$ 

For a system with Dead-space, part of the volume does not take part in the reaction. The overall volume (V ) is the summation of the dead-space ( $V_D$ ) and the active volume ( $V_A$ ).

$$V = V_D + V_A$$

Where the new observed MRT is:

$$\tau_{obs} = \frac{V - V_D}{v}$$

And then comparing the ratio of the two MRTs:

$$\frac{\boldsymbol{\tau_{obs}}}{\boldsymbol{\tau}} = \frac{(V - V_D)/v}{V/(v)}$$

Commented [WU73]: AVERAGE IS NOT THE SAME AS THEORETICAL

Commented [WU74]: These three in a table

$$\frac{\tau_{obs}}{\tau} = 1 - \frac{V_D}{V}$$

$$\tau_{obs} = \tau \times (1 - \frac{V_D}{V})$$

The last line shows that for a reactor with dead-space  $\tau_{obs}$ , the observed MRT, will be smaller than the theoretical MRT. The last four expressions are repetitive and too elementary.

As a summary, the following has been shown

$$\tau_{Dead-Space} < \tau_{Theoretical} < \tau_{By-pass}$$

### 2.3.4 Hold-back and Segregation

Danckwerts had described two additional quantities of interest to describe the RTD: The Hold-back (H) and the Segregation (S)[42]. These quantities are related and both are observed from the Distribution Function (F(t)).

The Hold-back represents the degree of which some elements of a fluid spend more time in a reactor than average. It is defined as:

$$H = \int_{\theta=0}^{\theta=1} F(\theta) d\theta \tag{2.3}$$

This quantity is represented as the area under the curve (Figure 2.12) of the dimensionless F(t) between  $\theta$  = 0 and  $\theta$  = 1. The two values of the shaded areas are the same due to the symmetry. The value of H will vary from 0 for plug-flow conditions to 1 for total dead-space. The value for H will be e<sup>1</sup> (  $\approx$  0.3679) for the ideal CSTR.

### $e^1 \approx 0.3679$ is wrong AND e= 2.71828.

The quantity of segregation (S) on the other hand, represents the deviation from perfect mixing from a CSTR. The value is found from superimposing the plot of F(t) with that of the ideal CSTR which is  $F(\theta) = 1 - e^{-\theta}$  (Figure 2.13). There is a second case which represents a reactor with dead-space were the reactor F(t) proceeds (Or precedes?) the ideal CSTR F(t) (Figure 0.14). This provides another test for the presence of dead-space. The two shaded areas again represent the same value due to the symmetry

Commented [WU75]: Dead Space has no hyphen

Commented [WU76]: AVERAGE IS NOT THEORETICAL!!!!!!!

Commented [WU77]:

Commented [WU78]: ....fraction of a liquid

(both Figure 2.13 and Figure 0.11). To show that is represents a deviation from the ideal conditions, the value is taken to be as negative. The quantity varies from e<sup>-1</sup> for plug-flow to -1 for entirely dead-space.

### 2.4 Ideal Models

The first step to modeling the behavior of idealized flow is utilizing the first principles of chemical engineering and performing a mass balance across the reactor. This procedure was outlined by Salmi[44]. Performing the Macroscopic Molar balance for the system obtains:

Alternatively, it can be represented mathematically as:

$$\frac{dN_i}{dt} = -\Delta[\dot{N_i}] + V \sum_{j=1}^{N_R} R_{gen}, ij$$

**EXPLAIN IN DETAIL THE MATERIAL BALANCE (2.5).** 

Commented [WU79]: EXPLAIN ALL THE PARAMETERS . WHAT IS 1?

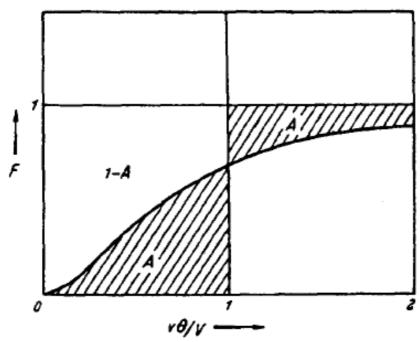


FIGURE 0.13: HOLD-BACK[13]

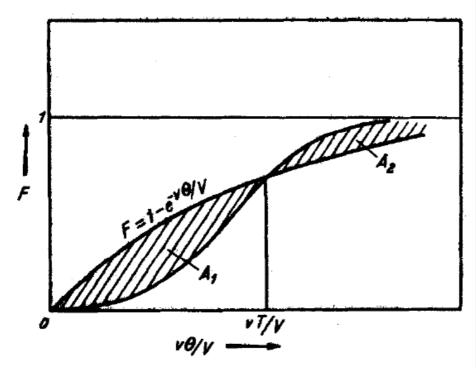


FIGURE 0.12: SEGREGATION QUANTITY (S)[13]

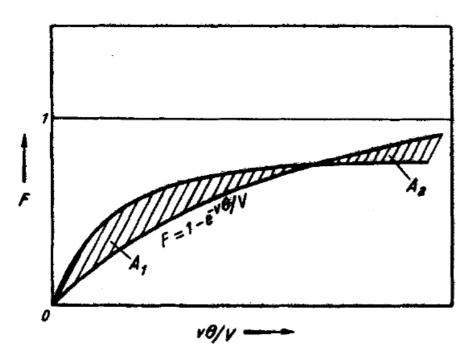


FIGURE 0.14: SEGREGATION QUANTITY (S) WITH DEAD-SPACE[13]

### FIGURE 2.13 is placed before Figure 2.12.

Where  $N_i$  represents the molar amount of a substance entering the reactor, V represents the volume of the reactor,  $R_{gen,ij}$  represents the sum of all reactions. The molar amount can be represented as concentration by the definition of molar concentration.

### **EXPLAIN THE DIAGRAMS!! WHAT ARE A1, A2, A**

$$C_i = \frac{N_i}{V} \tag{2.6}$$

$$N_i = C_i V (2.7)$$

Substituting equation (2.7) into equation (2.5) to obtain:

$$\frac{dN_i}{dt} = -\Delta[N_i] + V \sum_{j=1}^{N_R} R_{gen}, ij$$
 (2.5)

Commented [WU80]: EXPLAIN WHAT ARE A1, A2, A.

Commented [WU81]: EXPLAIN ALL THE PARAMETERS .

$$\frac{d(C_i V)}{dt} = -\Delta \left[ \mathbf{C}_i V \right] + V \sum_{j=1}^{N_R} R_{gen}, ij$$
 (2.8)

Equation (2.8) can be simplified with the assumption of a constant reactor volume, <u>V</u>, and constant flow rate, <u>V</u>, to become:

So, the <u>reactor volume V</u> is the same as the <u>constant flow rate</u> <u>V</u>?

$$V\frac{dC_i}{dt} = -v\Delta[C_i] + V\sum_{j=1}^{N_R} R_{gen}, ij$$
 (2.9)

Dividing both sides by the molar flow rate v do you mean v????????:

$$\frac{V}{v}\frac{dC_i}{dt} = -\Delta[C_i] + \frac{V}{v}\sum_{j=1}^{N_R} R_{gen}, ij$$
 (2.10)

Your equations are full of mistakes and very difficult to follow. Edit them and make them consistent.

Utilizing the following definition of the mean residence time:

$$\tau = V/v \tag{2.11}$$

Be consistent in page 19 you call  $\tau$ , theoretical RT, now you call it mean RT. AGAIN, MEAN IS NOT THE SAME AS THEORETICAL

In addition, substituting it back into equation (2.9):

$$\tau \frac{dC_i}{dt} = -\Delta [C_i] + \tau \sum_{j=1}^{N_R} R_{gen}, ij$$
 (2.12)

Commented [WU82]: A flow rate has nothing to do with a volume. !!!!!!

Commented [WU83]: Your equations are too confusing.

### 2.4.1 Continuous Stirred Tank Reactor

To find the response of a CSTR to a tracer injection, we can first simplify the mass balance in equation (2.10) by recognizing that for a tracer there is no reaction term. The equation can be further simplified due to no initial concentration of the tracer in the reactor at time t = 0. The tracer can then be treated as a pulse function ( $\delta$ ). **Define it.** 

Is this the Dirac Delta function? Or is it a first order DE? Then define it.

$$\tau \frac{dC_i}{dt} = -C \quad C = C_0, \ t = 0 \tag{2.13}$$

Rearranging the equation and integrating for the initial and final conditions,

becomes:

$$\int_{C_0}^{C} \frac{dC}{C} = -\frac{t}{\tau} = \ln \frac{C}{C_0}$$
 (2.14)

Where the concentration at any time can then be represented by the following:

$$C(t) = C_0 e^{-t/\tau} \tag{2.15}$$

### Residence Time distribution functions need to be normalized, the

C(t) function can be transformed to find the E(t) function which is the normalized probability function.

The function is defined such that: ALL THIS IS ORIGINAL OR TAKEN FROM A

REFERENCE?????

$$\int_0^\infty E(t)dt = 1 \tag{2.16}$$

Substituting the concentration function in the probability definition to obtain:

$$\int_0^\infty C(t)dt = 1 = \int_0^\infty C_0 e^{-t/\tau} dt = C_0 \tau$$
 (2.17)

For this expression to be balanced,  $C_0=1/\tau$  must be true. The normalized concentration is then:

$$E(t)_{cstr} = \frac{1}{\tau} e^{-t/\tau} \tag{2.18}$$

This idealized behavior is represented in Figure (2.12). The average value for the residence time of the probability function E(t) can be expressed as:

$$\overline{t} = \int_0^\infty t E(t) dt \tag{2.19}$$

Substituting the value for the probability function for the ideal CSTR as described in equation (2.18):

$$\overline{t}_{cstr} = \int_0^\infty \frac{1}{\tau} e^{-\frac{t}{\tau}} dt = \tau \tag{2.20}$$

This proves for the case of the ideal CSTR, the average residence time (t is NOT average residence time  $\overline{t}$  is) is equal to the residence time ( $\tau$ ) as it had been assumed. The general equation for the standard deviation ( $\sigma$ ) of a function f(t) is expressed as:

$$\sigma^2 = \int_0^\infty \left[ \overline{f} - f(t) \right]^2 E(t) dt \tag{2.21}$$

Where  $\overline{f}$  is the mean or average function.

For the special case of the ideal CSTR probability function:

## (t)

Time

FIGURE 0.15: E-DIAGRAM OF IDEAL CSTR FLOW

$$\sigma_{cstr}^2 = \int_0^\infty \left[\overline{t} - \tau\right]^2 \frac{1}{\tau} e^{-t/\tau} dt = \tau^2$$

(2.22)

Where .....

Explain the difference between t,  $\overline{t}$  and  $\tau$ .

## Idealized CSTR RTD

FIGURE 0.16: F-DIAGRAM OF IDEAL CSTR FLOW

Time

This shows that the standard deviation for a CSTR is equal to the residence time. This implies that no distribution can be broader than the ideal CSTR.

The final step is the calculation of the Distribution Function which again can be calculated from the E(t) and equation (2.2). The values for the Ideal CSTR are displayed in Figure 2.15 and Figure 2.16 respectively. THIS SECTION IS NOT WELL EXPLAINED.

### 2.4.2 Plug Flow Reactor

For the idealized case of Plug Flow Reactor, you could obtained the response to a pulse by solving the transient PFR equation in a similar fashion as the CSTR but the solution can be simply obtained by following the pulse down the reactor length.[49] The  $\delta$ (0) function moves down the length of the reactor without broadening because of the assumption of perfect plug flow behavior in which no mixing takes place. The tracer then travels the full length of the reactor and exits at the mean residence time, which can be simply expressed as the length of the reactor divided by the velocity of the fluid as explained in equation (2.11). Since no change in behaviour from injection, the RTD can be represented by the same function from the injection (the  $\delta$ (0) function). **DEFINE the Dirac Delta** function and why you need to use it here?

Commented [WU84]: These are no values but a figure.

Commented [WU85]: Rewrite this section.

Commented [WU86]: grammar

Commented [WU87]: ....there is no change in the flow profile from injection

Commented [WU88]: Define the Delta Function

$$E(t)_{PFR} = \delta(\tau) \tag{2.23}$$

# Time

FIGURE 0.17: F-DIAGRAM OF IDEAL PFR FLOW

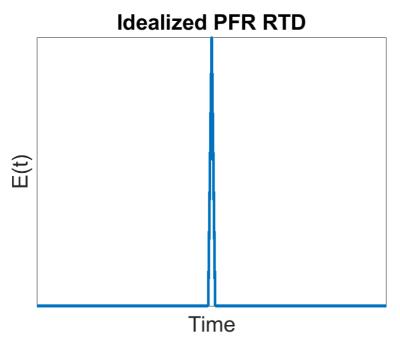


FIGURE 0.18: E-DIAGRAM OF IDEAL PFR FLOW

The standard deviation for a PFR can then be calculated from equation (2.21) but again since there is no mixing it is easy to understand that the following is true:

$$\sigma_{PFR} = 0 \tag{2.24}$$

#### 2.5 Real Reactor Models

#### (This section should be before CSTR, AD, and PFR)

Real Reactor Models are mathematically generated equations used to fit Residence Time Distribution curves. In this way, we can test different model parameters against the true behaviour of a reactor. The simplest of Real Reactor models are the single parameter models, which include the CSTR in series, and the axial-diffusion models (referred to as axial-dispersion models). More complicated models exist but their usefulness has diminishing returns as they become more complex with additional parameters.

#### 2.5.1 CSTR in Series

The CSTR in series, also referred to as the tank in series model, models the flow from one CSTR to another for a set number of CSTRs (Figure 2.19). These individual CSTRs are modeled by the ideal CSTR with identical reactor volumes. With an increase in the number of CSTR in series from one to infinity, the flow behaviour deviates from the ideal CSTR to the ideal PFR. This variation in the flow dynamic profile provides a great flexibility to the system. The algorithm is based on the following equations:

$$E(\theta) = \frac{N(N\theta)^{N-1}}{(N-1)!} e^{-N\theta}$$
 (2.25)

#### This equation is not derived or explained?

Figure 0.20 shows the effect that changing the design parameter N, the number of CSTRs in a series, has on the RTD. A Matlab code was created that employs the algorithm along with a vector of different values or N (From 1 to 20). This model has been compared to different tracer experiments.

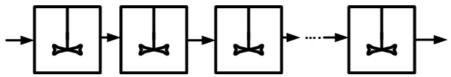


FIGURE 0.19: CSTR IN SERIES SCHEMATIC

Commented [WU89]: ..reactor in series because a tank is not a reactor is only a reservoir.

Commented [WU90]: reactors

## **CSTRs in series Model RTD**

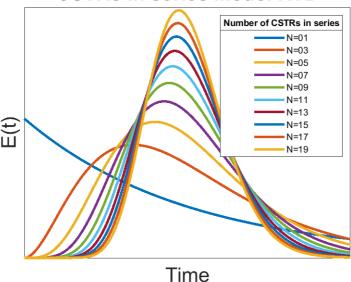


FIGURE 0.20: RTD FOR CSTRS IN SERIES FOR DIFFERENT NUMBER OF REACTORS CSTRS

# Explain what E(t) becomes as $t\rightarrow 0$ . What is the relevance in tracer methods.

#### 2.5.2 Axial Dispersion Model

The Axial Dispersion model starts with the foundation of the PFR but adds a degree of backmixing. The magnitude of the backmixing is independent of the position within the reactor. The concentration profile can be described by the following **time dependent**, second order **partial differential equation:** 

$$\frac{\partial C}{\partial \theta} = \left(\frac{D}{uL}\right) \frac{\partial^2 C}{\partial z^2} - \frac{\partial C}{\partial z}$$
(2.26)

The following equation describes the RTD for small levels of dispersion. This is a simplification and not a full solution to the differential. It should be noted that the equation that is within 5% accuracy when  $(\frac{D}{uL}) < 0.01[3]$ .

Commented [WU91]: Derive and read on the axial dispersion model.
What is differential?

You throw a DE without explaining the variables or the meaning of them. Explain the significance and use of the dimensionless number  $\left(\frac{D}{\nu L}\right)$ 

$$E(\theta) = \frac{1}{\sqrt{4\pi(\frac{D}{uL})}} \exp\left[-\frac{(1-\theta)^2}{4(\frac{D}{uL})}\right]$$

(2.27)

As the model has a second order **PARTIAL** differential **equation**, it requires two boundary conditions, **and the initial condition if time dependent**, to solve. The boundaries are taken as the inlet and outlet of the reactor. Each boundary can either be considered open or closed (Figure 2.22). Open signifies undisturbed dispersion as it passes the boundary while closed signifies plug flow outside of the boundary. The two situations of greatest

# Dispersion Coefficent D=00 D=5.56e-02 D=1.11e-01 D=2.22e-01 D=2.78e-01 D=3.38e-01 D=4.44e-01 D=5.00e-01

FIGURE 0.21: RTD FOR SMALL DISPERSION

Is Figure 2.21 yours?

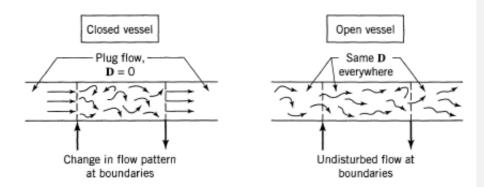


FIGURE 0.22: AXIAL DISPERSION BOUNDARY CONDITIONS[3]

interest are the open vessel (open/open) and the closed vessel (closed/closed). The closed vessel condition cannot be solved analytically but it can be solved numerically. The open vessel can be described by the following equation and Figure 2.23:

$$E(\theta_{\infty}) = \frac{1}{\sqrt{4\pi \left(\frac{\mathbf{d}}{\mathbf{u}L}\right)}} \exp\left[-\frac{(1-\theta)^2}{4\theta \left(\frac{D}{uL}\right)}\right]$$
(2.28)

#### WHAT IS d above? The Mass diffusion coefficient?

The difference observed from going from the low dispersion model to the open dispersion model is a shift to the left with a longer tail. The low dispersion model exhibits symmetry across the time axis. The solutions have been published for the boundary conditions open/closed and closed/open.[50]

#### 2.5.3 Enhanced CSTR in series

The Enhanced CSTR in series model is based on the original model but it includes two additional parameters [51]. The model represents a series of CSTRs in series in which a portion (1-n) will bypass the specific CSTR (Figure 2.24). This variable ranges in value from 0-1 where n = 1 is 100% likely to enter the CSTR. The probability for bypass is equal for each CSTR in series. The second parameter M represents the opportunity for dead-space within each CSTR. Just as in the previous parameter, the probability is the same at each CSTR and the range is from 0 to 1. These additional parameters significantly increase the complexity of the model. To solve this model a  $N \times n \times M \times \theta$  grid needs to be created. The model is described by the following equation:

Commented [WU92]: Why ???

Commented [WU93]: WHAT IS AN ENHANCED CSTR?

Commented [WU94]: Very hard to follow

$$E(\theta) = \frac{Nn}{M} \sum_{i=1}^{N} \frac{N! e^{-\frac{nN\theta}{M} \left(\frac{Nn\theta}{M}\right)^{i-1} n^i}}{(N-i)! i! (i-1)!} + (1-n)\delta(\frac{Nn\theta}{M})$$

# Equation (2.29) above means nothing if you fail to explain every symbol

(2.29)

The model equation is not very programming friendly. The summation term requires the use of a for loop in Matlab which prevents the function from becoming 100% vectorized. This will significantly increase the required **computational time** for simulation. The application of a four dimensional grid also requires a lot of system memory reducing the resolution for the parameters while also increasing the computational time.

#### IS THE FIGURE BELOW YOURS?

## **Open Vessel Disperssion**

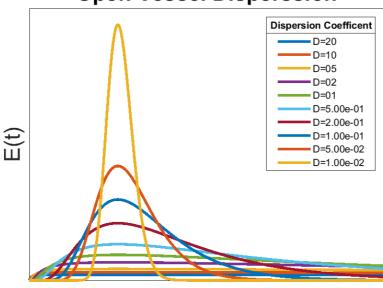


FIGURE 0.23: RTD FOR OPEN VESSEL DISPERSION

Time

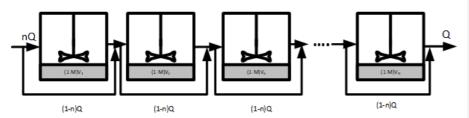


FIGURE 0.24: ECSTR SCHEMATIC

Is the above figure yours? If not, where is the reference? EXPLAIN every parameter N, n,

## ECSTRs Model(n=1,N=2)

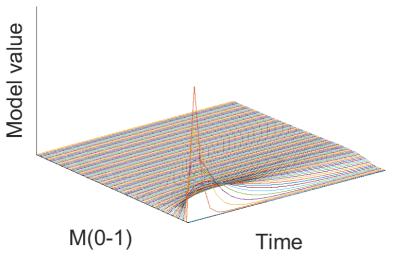


FIGURE 0.25: ENHANCED CSTR IN SERIES EFFECT OF M

## 2.5.4 n-CSTR Model

One of the major limitations of the CSTR in series model is the reliance on the factorial of (n-1). This term limits the application of this model to natural numbers of n. Martin overcame this obstacle with the

Commented [WU96]: Who is this guy?????

Commented [WU97]: You mean Martin-Dominguez?

application of the Gamma function  $(\Gamma(n))$ [52][53]. The Gamma function has been defined by Eular as the following:

Commented [WU98]: YOU MEAN EULER ?????

$$\Gamma(n) = \int_0^\infty x^{n-1} \cdot e^{-n} dx \tag{2.30}$$

## If the mathematical tools and their application are not described even in the Appendix don't use them.

Where the following conditions are also satisfied:

$$\Gamma(0) = \Gamma(1) = 1$$

$$\mathbf{n} \cdot \Gamma(n) = \Gamma(n+1) \forall n \in \mathbb{R}$$

$$\Gamma(n) = (n-1)! \forall n \in \mathbb{N}$$

There are two advantages to this modification: the representation of value between real numbers (such as values between 1 and 2 when neither of them quite fit well), and the representation of systems with by-passing were N < 1.

Figure 0.27 outlines the different Residence Time Distribution functions for different values of N using the n-CSTR Model. The n-CSTR Model (also referred as the Extension to Tank in Series (ETIS))

## Enhanced CSTRs in series Model(M=1,N=2)

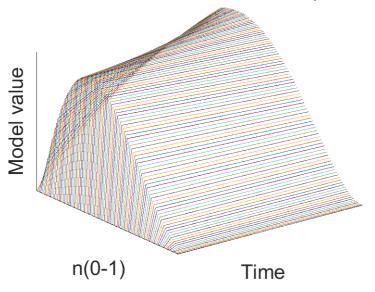


FIGURE 0.26: ENHANCED CSTR IN SERIES EFFECT OF N

Commented [WU99]: REFERENCE?

## **Generalized N CSTRs Model**

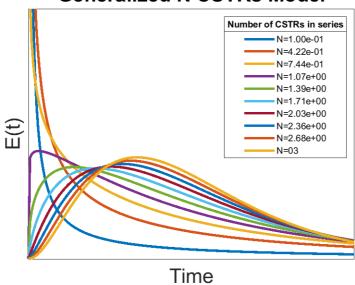


FIGURE 0.27: RTD FOR N-CSTR MODEL AT DIFFERENT NUMBER OF CSTRS

Commented [WU100]: REFERENCE?

approaches the PFR when the value of  $N \to \infty$ . Similarly, the model is equal to the ideal CSTR when N = 1. The unique behaviour of this model allows the demonstration of the two extreme ideal models along with a model exhibiting bypassing when 0 < N < 1.

#### 2.6 Computational Fluid Dynamics

# Is this experimental work that you include with the literature survey? If so where are your references?

There have been many interesting developments in the area of Computational Fluid Dynamics (CFD) over the last decade. CFD models have the potential to meet some of limitations of RTD. The RTD can provide insight on dead-space and by-pass channeling but it does not provide any dimensional information. The basis of CFDs is the simulation of the Navier-Stokes equation extended over the three dimensions of the reactor. Research has shown that a CFD can develop a series of **steady moment** transport equation to derive the moments of the RTD without the need for a tracer experiment[54] CFDs are not a perfect solution, there are still parameters that need to be evaluated such as: approach, discretization scheme and turbulence model[55].

Materials and Methods.

**Chapter Number?** 

## 3.1 Construction of the STAR reactor

The original STAR reactor, developed by Dr. Maryam Reza and Dr. Manuel Alvarez Cuenca in 2016[2], was deconstructed with some of the parts used for the study of an alternative reactor in another study. The components of the STAR reactor required reassembly following the process flow diagram outlined in Figure 3.1.

#### 3.1.1 Tracer Selection

It is important that the tracer selected acts as a good representation of the fluid flow, thus the tracer selection process is paramount. It is important that the tracer exhibits the following characteristics[45]:

- 1. The tracer should be stable and conserved
- 2. The analysis for the tracer should be convenient, sensitive, and reproducible
- 3. The tracer should be inexpensive
- 4. The tracer should not be absorbed on or react with the surface of the vessel
- 5. The tracer should be chemically and physically similar to the fluid flow.

Commented [WU101]: You miss the Chapter numbers.

**Commented [WU102]: NO.** A tracer is a substance a flow is a form of flow. REWRITE THIS SENTENCE

Commented [WU103R102]:

Commented [WU104]: WHAT IS A CONSERVED TRACER?

Commented [WU105]: Rewrite section 3.1.1.

Traditionally the tracer has been nonreactive but a decaying tracer can be corrected for.[50] There has been research in the use of reactive tracers for long term model monitoring; however, it doesn't allow for the determination of the RTD.[48] The benefit of a reactive tracer is that a process reagent can act as the reactive tracer so no additional work is required.

Missen suggests the following additional precautions when performing a tracer experiment[45].

- Inject properly: If the velocity profile at vessel inlet is at, introduce tracer uniformly across the cross section. If it is not at, introduce tracer proportional to the flow rate.
- Measure properly: Average over all flow rates. This is called the mixing cup measurement.

Commented [WU106]: That is, a reagent can be a tracer.

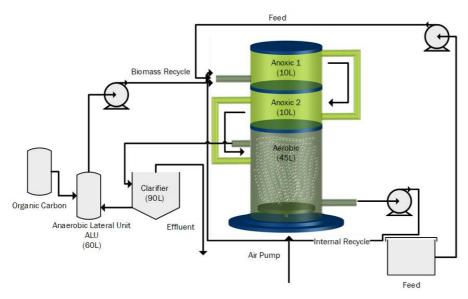


FIGURE 0.1: STAR VERTICAL BIOREACTOR: PROCESS FLOW[6]

Through the field of water engineering, many different tracers are available. Some of the different possible tracer technologies are summarized in Table 2. The tracer criteria are summarized in Table 3.

Method	Principle
Conductivity	Electrical Conductivity
Photometry	Light absorbance (visible or ultra-violent)
Mass Spectroscopy	Different mass numbers of components
Para-magnetic Analysis	Para-magnetic properties of compounds
Radioactivity	Radioactive radiation
Gas Chromatography	Adsorption of a compound on a carrier material
Liquid Chromatography	Adsorption of a compound on a carrier material

TABLE 2: COMMON ANALYTICAL METHODS FOR TRACER EXPERIMENTS[44]

After the type of tracer has been selected, it is important to select what type of signal  $\frac{1}{1}$  would like to simulate. The first and simplest signal is the Dirac Signal ( $\delta$ ) also known as a pulse signal. This signal requires the injection of a single volume of injectable material at time t = 0 with the concentration of  $C_0$ . It has the major advantage that it only requires a small amount of tracer. It also has

a small impact on the process operation. Some trade-offs exist as it can be difficult to produce the perfect pulse. The full amount of the tracer needs to be injected at an instance. It can also make it di cult to perform a mass balance for the tracer.[45]

Commented [WU107]: You mean "instant"?

In some cases, a step input is preferred where a set constant flow rate of tracer is continuously added to the system. This can be performed by a "step up" or a "step down" in tracer concentration and This creates a system method that is easier and simpler to perform a mass balance. For as well as being easier to achieve, . The opposite of the pulse function is also true. It requires much more tracer element and it is more likely to affect process operation [45].

Commented [WU108]: "larger amounts of tracer"

Commented [WU109]: WRITE A LIST OF ADVANTAGES AND DISADVANTAGES OF EACH METHOD.

A periodic signal or a random signal can also be used; however, these signals are much more complicated to generate then a step or a pulse. The random or periodic signals are also more difficult to interpret. The pulse method was selected due to the simplicity and minimal requirement for tracer.

Commented [WU110]: GRAMMAR

There have been some interesting developments in the application of alternative tracers. Ahnert studied storm water events with cold water as a tracer signal for a Waste Water Treatment Plant (WWTP)[56]. This would be a very simple and cost-efficient method for performing tracer experiments. Reactive tracers are another potential avenue such as the experiments performed by Braun[57]. The WWTP under study experiences fluctuations of ammonia and oxygen concentrations at night due to an unresolved issue in the process. Braun was able to use these fluctuations as a randomly generated tracer signal. The disadvantages of a reactive tracer include uncertainty of the measurement device and a lower detection limit.[58]

Commented [WU111]: Who did? Where?

A solution of sodium chloride was selected as a tracer. It is frequently used in industry as it behaves similarly to wastewater. The tracer is also very cheap and easy to obtain. The tracer however can not be used for wastewater - it will be absorbed by microbes - but it is appropriate for clean water. Very little system modifications would be required to experiment with wastewater and a Lithium Chloride tracer. Lithium Chloride has the advantage of low absorption rates in the activated sludge. There are some concerns about the toxic effect of Lithium Chloride on aquatic life including effects on algae and minnow larvae[59].

Commented [WU112]: Write in a table the kind of tracers and the costs, flexibility, pros and cons.

#### 3.1.2 Sensor Selection

The measurement of conductivity is not 100% standardized. There are a few different units measurements but one of the most common ones is the Micro Siemen per centimeter ( $\mu$ S/cm). Often the /cm is omitted **why?** It was determined that the maximum range required for saturated sodium chloride solution would be about 10,000  $\mu$ S/cm[60]. A saturated solution of Lithium chloride was found to be only slightly higher.

Technology	Criteria			
	Price	Sensitivity	Industrial Application	Operation
Conductivity	Cheap	Wide	Common[48], [51], [57], [61]–[64]	Continuous
Photometry	Cheap	Wide	Common[62], [65]–[67]	Continuous
Mass Spectroscopy	Expensive	Wide	Common	Discontinuous
Para-magnetic	Cheap	Wide	Common	Continuous
Radioactive	Expensive	Wide	Uncommon[46]	Continuous
Chromatography	Expensive	Wide	Uncommon	Discontinuous

TABLE 3: TYPES OF TRACER SENSORS TECHNOLOGIES CRITERIA

The CDCE-90-1 conductivity cell was chosen for this experiment as it was provided by a recommended supplier and it was capable of covering the required conductivity range (10-10000 S=cm). The range available for a cell is dependent on the cell constant. A higher cell constant has a higher range but it will be less sensitive on the lower limit. The CDCE-90-1 was able to handle the highest conductivity reading of the saturated tracer solution and the lowest possible value as the conductivity of tap water, which is  $\approx 300~\mu\text{S/cm}$ .

#### 3.1.3 Sensor Placement

One of the larges t tasks in assembling the tracer experiment was deciding how the sensors would fit into the reactor. The current sensors are submersed in the reactor, attached through the walls. This would not be acceptable for the conductivity sensors as this configuration assumes perfect mixing and constant parameters in each section. The entire purpose of the tracer experiment is to move from this simplified assumption into a model that better describes the true mixing dynamics.

It was clear that the sensors had to be attached in-line with the piping as per the suppliers' instructions (Figure 3.2). One consideration that was made was the liquid level in the piping. The sensor itself has a hole, for fluid flow, with a wire across. It was important that the sensors remained submerged in the fluid. For some of the sensors this require no modification as their location remained under the liquid level. The two sensors on the top of the reactor (Sensor 1 and 2 on Figure 3.4) required the liquid to be held back in order to raise the liquid level. The first sensors used a cork (Visible in Figure 3.5) while sensor two used a piece of rubber that was folded into the piping and not visible.

Commented [WU113]: YOU DO NOT INCLUDE IT IN TABLE #

Commented [WU114]: NOT CLEAR TO ME !!!!!

Commented [WU115]: IN WHAT PIPING?

Commented [WU116]: THE SENTENCE IS INCOMPLETE.

Commented [WU117]: THE FIGURE MUST BE NEAR THE TEXT.

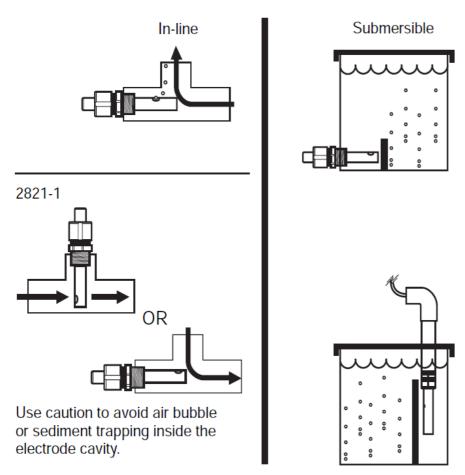


FIGURE 0.2: SENSOR ALIGNMENT[39]

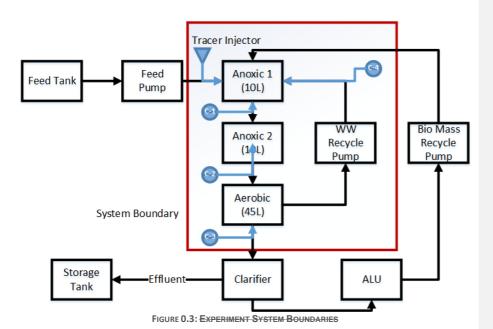
#### 3.1.4 Instrumentation and Methodology

The original series of sensors were used to ensure the same operating conditions as in the **previous study**. The experiment required an additional series of conductivity sensors in the original instrumentation setup. The Data Acquisition System (DAS) was flexible enough to accommodate the additional sensors. The conductivity sensors were strategically placed through the process to enhance the information collected while reducing costs by limiting the number of sensors. The Process and Instrumentation Diagram (P&ID) is outlined in Figure 3.4.

The Data Acquisition System (DAS) was connected to a local computer that ran Lab-View to monitor the sensor data. Lab-view would record the sensor data for all the sensors and output excel spreadsheets that were used for analysis.

Commented [WU118]: WHAT PREVIOUS STUDY? REFERENCE.

Commented [WU119]: PLACE THE FIGURE NEXT TO THE TEXT



FLOW DIAGRAM OF THE EXPERIMENTAL UNIT

#### 3.1.5 Tracer Injector

The commercial availability of injectors is limited On the topic of injector systems, there are limited commercial products. One such product is the injector port used in medicine for different intravenous therapy (Figure 3.6). Researching such an injection port as well as obtaining one is difficult as it is highly regulated. The decision was made to make a custom solution for the problem.

There were two different tracer injector trials. The first trial utilized a t-connection, a rubber stopper, a syringe and a needle (Figure 3.7). The injector port design joined the t-connector and the rubber stopper. The tracer itself would be injected in a 10 mL syringe with a needle into the injection port. The T-connection was spliced into the feed line from the feeding tank to the first anoxic stage. The connector was placed close to the reactor in order to reduce any amount of lag introduced by the injection process.

The T-connector was a three-sided barbed connector with a 3/4 inch size that was purchased at a local Home Depot. The rubber stopper and the needle were generously supplied from the Chemistry department at Ryerson University. The syringe was provided from the Water treatement Technology lab at Ryerson University.

Commented [WU120]: Make your text simple, clear, and brief.

Commented [WU121]: YOU PLACE FIGURES BUT DON"T EXPLAIN WHAT THEY ARE.

**Commented [WU122]:** WHY DO YOU PLACE IT SO FAR AWAY FROM THE TEXT??????

Commented [WU123]: PLEASE LET US KNOW WHAT WAS THE PRICE?? IF IT IS VERY LOW TO MENTION IT IS NOT GENEROUS, IF IT IS VERY EXPENSIVE THEY WILL BE REIMBURSED

TO MENTION THE SERYNGE AND THE RUBBER STOPPER IN THESE EXPERIMENTS APPEARS FARFETCHED. What percent of the total MASc is the stopper & syringe is ?

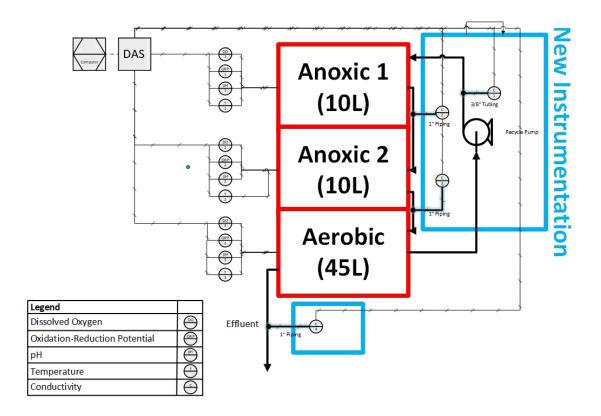


FIGURE 0.4: STAR REACTOR: PROCESS AND INSTRUMENTATION DIAGRAM



FIGURE 0.5: SENSOR #1 WITH A PIECE OF CORK?



FIGURE 0.6: INTRAVENOUS THERAPY INJECTOR PORT[39]

Stream	Flow rate (L/hr)
Feed	10
Internal Recycle	20
Recycle Sludge	15

TABLE 4: VERTICAL REACTOR OPERATING CONDITIONS[1]

There was a 3/4 inch hole bored partially into the stopper that allowed the stopper to fit onto the t-connector. The theory behind **the stopper** was that the thick rubber would act as a self-healing surface that would withstand multiple injections without any leakage. This had been proven mostly successful; however, it was found that the injector did not provide enough tracer solution to provide any measurable data at the end of the reactor. This had led to the development of the second injector design.

The second injector design was much simpler; getting rid of the injector port all together (Figure 3.8). A larger 50 mL syringe was connected directly into the t-connection with a small length of tubing. The length of tubing was minimized in order to reduce any lag time and any dead space that would reduce that amount of tracer injected. Initially a rubber band was tied around the syringe to prevent back- flow into the injector but the pressure in the line was found to be insufficient to cause this effect.



FIGURE 0.7: TRACER INJECTOR TRIAL 1

Commented [WU124]: But a rubber stopper is not such an extraordinary device.

Commented [WU125]: Even more simple ???

Commented [WU126]: FIGURE 3.8 explains nothing.

Commented [WU127]: The picture in 3.8 is difficult to interpret.

Different volumes of tracer were tested and it was found that 50 mL was sufficient. The operating conditions were maintained the same as literature values to ensure consistency (Table 4).

Commented [WU128]: GIVE NUMBERS . "DIFFERENT" IS **NOT GOOD ENGINEERING** 

#### 3.2 Data Analysis

## 3.2.1 Conductivity versus Concentration (of what?)

The assumption that the conductivity of a tracer solution was linearly related to concentration of such solution was made. This assumption simplifies the creation of the RTD diagrams, as the conductivity measurements would require an additional conversion step to concentration.

Some of the conductivity sensors had shown strong evidence of wear with the formation of rust as evident in Figure 3.9 and Figure 3.10. Performing this assumption also had the additional benefit of  $eliminating \ the \ requirement \ of \ continuously \ re-calibrating \ the \ sensors. \ The \ sensor \ that \ exhibited \ wear$ still produced a reading but it would be inconsistent with other sensors. When transforming the readings into the dimensionless E(t) charts, any deviation between sensors would be removed. Only the sensors consistency with itself could provide a problem.

Commented [WU129]: PLACE ARROWS IN THE PICTURES POINTING THE RUSTING SPOTS

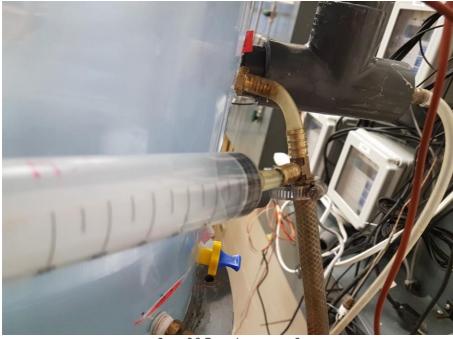


FIGURE 0.8: TRACER INJECTOR TRIAL 2



FIGURE 0.10: FORMATION OF RUST



FIGURE 0.9: THE EFFECT OF RUST

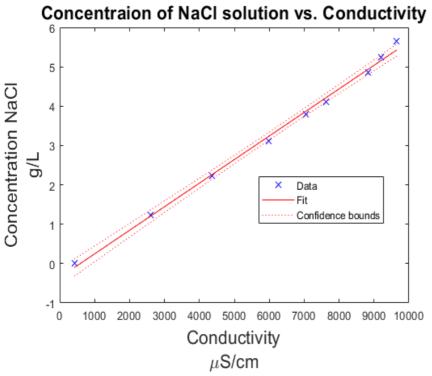


FIGURE 0.11: CONCENTRATION VS. CONDUCTIVITY

#### SPELL "CONCENTRATION" IN THE GRAPH

between the concentration of sodium chloride in tap water and conductivity. Sodium chloride acts as the tracer in the experimental unit (vertical bioreactor). A beaker with tap water was place on a hot plate with a magnetic stirrer. There was no requirement to use distilled or de-ionized water as the main feed in the reactor was tap water. The average conductivity would never be in the range of de-ionized water. With the use of a laboratory scale, small amounts of laboratory grade sodium chloride was added to the beaker. It is important to note that the behavior of laboratory sodium chloride is different than regular table salt. Table salt includes an anti-caking

Commented [WU130]: CONCENTRATION
Commented [WU131R130]:

Commented [WU132]: Explain your determination of linearity of conductivity with water.

Commented [WU133]: spelling

Commented [WU134]: 'a'

Commented [WU135]: Explain why a hot plate.

Commented [WU136]: draw A DIAGRAM WITH THE EXPERIMENT.

Commented [WU137]: Give figures.

Commented [WU138]: WHAT IS SMALL. FIGURES !!!!!!!!!!!

agent that prevents clumping and enhances ease of pouring.[68] Without the anti-caking agent, laboratory sodium chloride is much more difficult in measuring equal weights. The actual sensors used to develop the RTD diagrams were used to ensure consistency. A laboratory conductivity meter would have provided more accurate results of the relationship but the main interest is the effect on the specific sensors that are used.

Into total, eight different samples of sodium chloride that were added to the solution for nine different conductivity measurements. The experiment continued to a conductivity reading of 10,000 µS/cm as that is the maximum reading for the sensor and very close to the upper limit for the solubility of sodium chloride in water. The results of the experimentation can be found in Figure 3.11. It is evident of a strong linear relationship as the R² value for the linear interpolation is 0.996. This justifies the assumption that they are directly related.

Commented [WU139]: SPELLING

Commented [WU140]: REWRITE THIS SENTENCE.

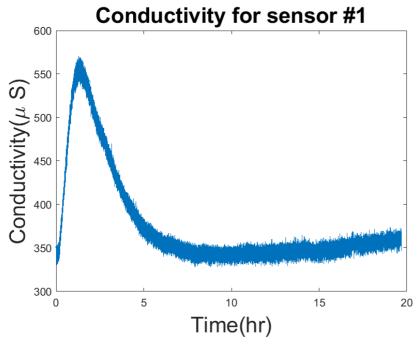


FIGURE 0.12: SAMPLE CONDUCTIVITY GRAPH

#### 3.2.2 Transformation to Population Density Function

#### Performing t

The tracer experiment produces results in a spreadsheet of the different conductivity measurements taken at the sample time of every three seconds. These tables were **THEN** than expressed in a graphical format as observed in Figure 3.12.

A few issues need to be addressed to transform the sample results into the Population Density Function (DEFINE IT !!!!!!!). Since the conductivity of tap water is inconsistent and not equal to zero, the initial and final values need to be accounted for in order to transform the conductivity graphs into RTD graphs. This task was initial completed by simply subtracting the lowest value from every value. This did not provide satisfactory results as the initial and final conductivity values differed. The fouling of the sensors due to rust deposits likely causes this. A linear regression model was implemented to solve this problem from the first ten and the last ten data points. This was achieved in Matlab utilizing the function "fitlm". REPRESENT YOUR REGRESSION OF THESE POINTS IN THE APPENDIX.

Commented [WU141]: DO YOU KNOW WHAT A POPULATION DENSITY FUNCTION IS????

Commented [WU142]: "not uniform"

Commented [WU143]: Rewrite this sentence and explain it

There was a large amount of noise from the collected samples so a regression model was used to clean up the data. It was later decided that the Matlab function "filter" using a moving average was a better solution. The amount of points to be affected by the filter was chosen experimentally. The lowest value that significantly cleaned up the data, to the point where is looked like a smooth curve was selected.

The next step was to change the values from a function of the concentration to a probability. This is achieved with the following equation:

$$E(t) = \frac{C(t)}{\int_0^\infty C(t)dt} [1]$$
 (?????)

Where E(t) is .....and C(t) is......this formula based on the concentration of the tracer (C(t)) but it is also true for any function of concentration such as the previously proven conductivity. There are a few numerical methods to find the integral from a set of data points but the trapezoidal method was selected for its ease of use and because it is already built into Matlab and explained in Appendix...... The function can be describe by the following equation:

$$\int_{a}^{b} f(x)dx \approx \sum_{k=1}^{N} \frac{f(x_{k-1}) + f(x_{k})}{2} \Delta$$
 (3.2)

Experiments were performed with both the Simpson's rule and Simpson's 3/8 rule. There was minor differences in computational time and accuracy between methods especially with large data sets.

One advantage of using a concentration vs time graph is that the value of the integral across time is equal to the mass of tracer injected into the reactor. This provides an additional check to ensure that no tracer is absorbed by the <a href="system">system</a> or <a href="lost">lost</a>. The value obtained from an arbitrary measurement, such as conductivity, provides no such benefit.[3]

The Population Density Function graph can now be used to evaluate different flow models but this evaluation is even easier if the E(t) is transformed in dimensionless time ( $\theta$ ). This requires the values of time (t) being divided by the Mean Residence Time (MRT) which can be calculated by this equation. THIS IS THE FIRST MOMENT

$$\overline{t} = \int_0^\infty t E(t) dt \tag{3.3}$$

The transformation to dimensionless time requires the division of time by the MRT,  $\theta = \frac{t}{\overline{t}'}$  and the multiplication of the probability by the MRT,  $E(\theta) = E(t) \times \overline{t}$ . With this new plot,  $E(\theta)$  vs.  $\theta$ , models can be compared at the time constant  $(\tau)$  =1. This will significantly simplify the process.

Commented [WU144]: BUT I WANT TO SEE THAT YOU USE NUMERICAL METHODS NO MATLAB

Commented [WU145]: Simpson integration in the appendix

Commented [WU146]: Who cares about computational time in this case?

Commented [WU147]: This set is not so large

Commented [WU148]: What is the system?

Commented [WU149]: YOU DID NOT DEFINE IT.

Commented [WU150]: Where do you show it??????

Commented [WU151]: This to be placed early with the fundamentals.

In statistics, a moment generating function is used to determine the properties of a distribution function.[69] These functions are used to compare different distributions. The first moment represents the MRT. The second moment is the variance of a distribution which is defined by the following equation:

$$\sigma^2 = \int_0^\infty (t - \overline{t})^2 E(t) dt \tag{3.4}$$

The magnitude of the variance is an indication of the "spread" of the distribution.

The third moment is a quality referred to as the skewness. It is a measure of the extent that a distribution is skewed in one direction or the other in reference to the mean. It is observed as a tail. It is defined as:

$$s^{3} = \frac{1}{\sigma^{3/2}} \int_{0}^{\infty} (t - \overline{t})^{2} E(t) dt$$
 (3.5)

The first and the second moments are the most commonly used parameters to characterize a RTD function.

Commented [WU152]: These concepts should be earlier in the text.

#### 3.3 Model Testing

Different models were examined against the collected Dimensionless Population Density Function ( $E(\theta)$ ) for the different sections of the STAR reactor. These proposed models were evaluated with a custom Mat-lab function based on Root Mean Square Error (RMSE), which is described in equation (3.6).

RMSE = 
$$\sqrt{\frac{1}{n}} \sum_{j=1}^{n} (y_i - \hat{y}_i)^2$$
 (3.6)

Where.....

#### 3.4 Recycle Experiment

The tracer experiment was run without the **systems internal recycle**. The recycle sludge streamed was also turned off, as it would increase the overall volumetric flow-rate. This

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allowed the determination of the observed MRT through a single run. The effect of the addition of the recycle on the MRT can be observed. Optimization of the MRT by controlling the internal recycle rate can then be considered.

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#### 3.5 Characteristic Parameters

The data provided by the internal recycle testing allows for additional testing for dead-space and by-passing (as described in section 2.3.3). The theoretical mean residence time can be calculated by the following equation:

$$\tau = \frac{V}{v}$$

Where  $\tau$  is the theoretical mean residence time (hours), V is the total reactor volume (Liters) and v is the volumetric flow rate (Liters/hour). The total volume is the sum of the volumes of each section:  $V = V_{anoxic1} + V_{anoxic2} + V_{aerobic} = 10L + 10L + 45L = 65L$ . The volumetric flow rate was maintained at 10L = hr resulting in  $\frac{1}{2}\tau = 6.5hr$ s. The observed MRT was defined as  $\frac{1}{2}$  found with the following equation:

$$\overline{t} = \int_0^\infty t E(t) dt$$

#### YOU DEFINED THE MEAN BEFORE [2.19)

As a summary of section 2.3.3, the following relationship is true:

$$\tau_{Dead-space} < \tau_{Theoretical} < \tau_{By-pass}$$

The quantities of Hold-back (H) and Segregation (S) were also found as described in section 2.3.4. The values were obtained after finding the Distribution Function (F(t)) from the Population Density Function (E(t)). They are related from the following equation defined before:

$$F(t) = \int_0^\infty E(t)dt$$

#### THIS EQUATION WAS DEFINED BEFORE

All of these values were obtained with the use of Matlab scripts. You must present your own calculations. MATLAB does not show your understanding of Chem Eng only the routines of MATLAB.

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## : Results chapt.4

#### 4.1 Tracer Experiment

The following multiple plot (Figure 0.1) represents the raw data collected from the tracer experiment on December, 19, 2019. A sample of 50mL of saturated tracer solution was injected a few seconds after the initial sampling. The sampling rate was set to three seconds for the conductivity sensors. There is a plot for the each-conductivity at the recycle stream, ........... sensor, which represent the effluent of each stage of the reactor and the internal recycle. The graphs show the conductivity of the liquid flow trend of the tracer throughout the stages. There is Although some noise is observed in the raw data a but the general trend can be observed.

Repeated trials were performed to determine the The consistency of the dataresults. Was testing on. The overall RTD for the different trials are examined on Figure 4.2. There are some

As expected there are deviations between the trials as they exhibited different conditions (ex. tracer volumes) but their overall behaviour is consistent as shown in Table 5 which illustrates the error between each of the trials. This measurement of error will be used as a benchmark for the model testing. The first and second moments (Mean Residence Time and Variance) of the RTD for three different trials are summarized in Table 6.

Figure 4.3represents the dimensionless RTD function for the fourth sensor representing the effluent from the entire reactor. The plot exhibits a large thin peak followed by two wide but shorter peaks. The distance between each peaks is around 0.75 times the mean residence time. Figure (4.4) @@shows the dimensionless RTD for the raw data represented in Figure 0.1.

#### ORGANIZE THIS TABLE !!!!!!

Compared Trials	RSME		
Trial 1 and 2	0.206		
Trial 1 and 3	0.284		
Trial 2 and 3	0.364		
Average	0.285		

TABLE 5: ERROR BETWEEN DIFFERENT TRIALS, E(⊕)

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Commented [WU159]: Of concentration mg/L

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# Tracer Experiment Raw Data

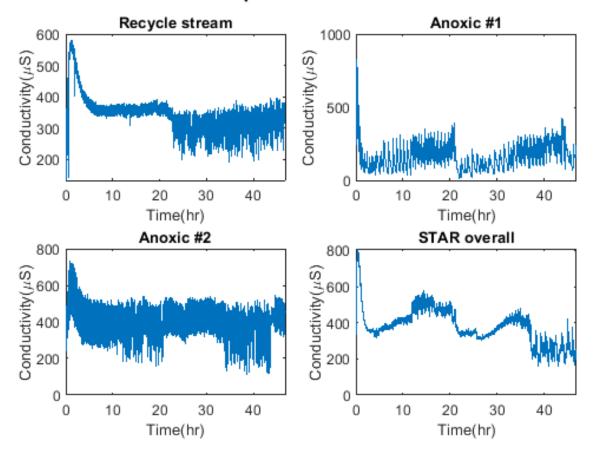


FIGURE 0.1:CONDUCTIVITY IN THE IN THE RAW DATA OF TRACER EXPERIMENT

SO MANY FIGURES AND NO TEXT!!!!!!!!

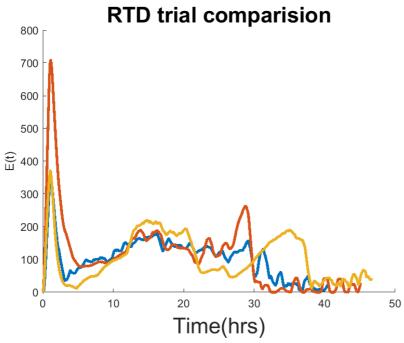


FIGURE 0.2: DIFFERENT RTD TRIALS FOR OVERALL REACTOR

AGAIN, EXPLAIN THOROUGHLY THIS GRAPH !!!!!!!

#### Mean Residence Time(hrs) Variance

Trial 1	16.9	94.7
Trial 2	14.7	113.5
Trial 3	21.2	141.6
Average	17.6	116.6

TABLE 6: RTD CHARACTERISTICS OF DIFFERENT TRIALS

ORGANIZE THIS TABLE, ORGANIZE YOUR THESIS.

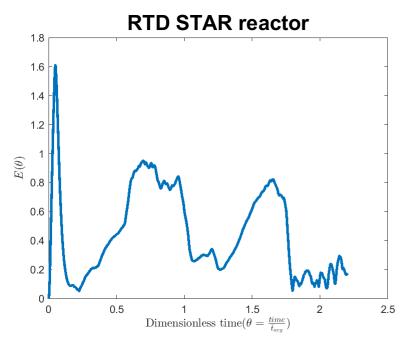


FIGURE 0.3: STAR REACTOR RESIDENCE TIME DISTRIBUTION FUNCTION

	CSTRR	PFR	Low D	DispOpen	CSTRS	Nth CSTR	E-CSTRS
Trial 1	0.27	92.47	0.18	0.25	0.25	0.25	0.20
Trial 2	0.27	75.05	0.30	0.37	0.27	0.27	0.26
Trial 3	0.37	107.43	0.29	0.32	0.32	0.32	0.30
Average (fit)	0.30	91.65	0.26	0.31	0.28	0.28	0.25

**TABLE 7: MODEL TEST SUMMARY** 

### **EXPLAIN THE DATA AND ORGANIZE TABLE 7**

YOUR TABLES AND FIGURES ARE VERY DISORGANIZED SO THEY CANNOT BE EVALUATED.

#### 4.2 Model Testing

Figure 4.5 demonstrates how the Ideal models fit the RTD for this trial while Figure 4.6 and Figure 4.7 test different real reactor models. The behaviour of RTD is closer to that of the Ideal CSTR than it is of the Ideal PFR. The difference in error between the two ideal conditions is on a factor of 3.

There are three reactor models in Figure 4.6 and two models in Figure 4.7. The real reactors are all better fits for the RTD than the previous ideal reactor models. Table 7 shows the average error measured for each of the models against three different experiment trials while Table 8 summarizes their parameters of best fit. The enhanced CSTR in series model shows the best fit for the data, but it is on the same scale as the ideal CSTR.

## **Tracer Experiment Transformed Data**

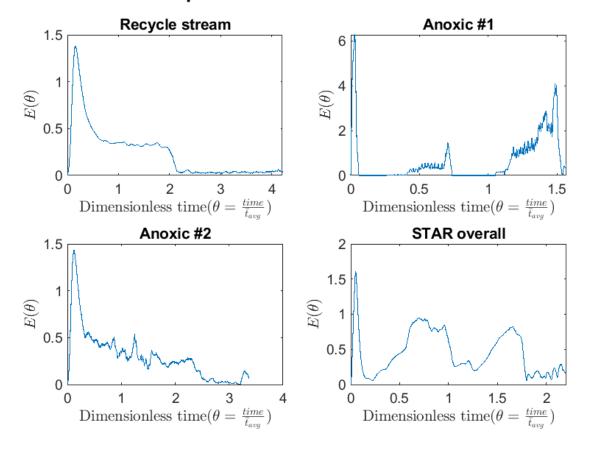


FIGURE 0.4: TRANSFORMED DIMENSIONLESS RESIDENCE TIME DISTRIBUTION

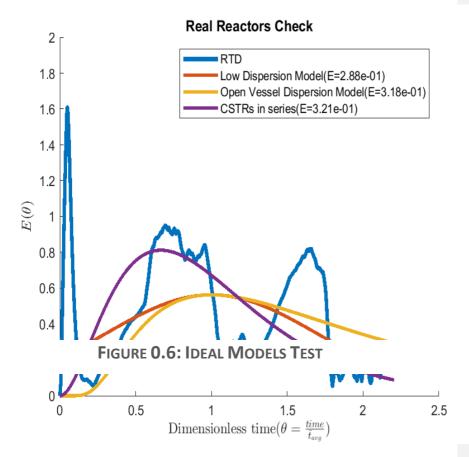


FIGURE 0.5: REAL REACTOR MODELS TEST

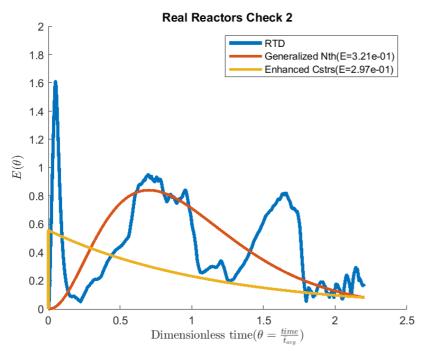


FIGURE 0.7: REAL REACTOR MODELS TEST CONT.

#### THE FIGURES AND TEXT OF THIS CHAPTER NEED TO BE REWRITTEN

	Low D	Open D	#CSTRS	#nthCSTRS	#ECSTRS	n min	M min
Trial 1	0.25	0.25	2	1.52	3	0.64	1
Trial 2	0.42	0.67	1	1	1	0.55	0.36
Trial 3	0.25	0.25	3	3.34	1	0.64	0.73
Average	0.31	0.39	2	1.95	2	0.61	0.7

TABLE 8: MODEL OPTIMAL PARAMETERS

#### **NO OBSERVATIONS OR ANALYSIS OF THE DATA????**

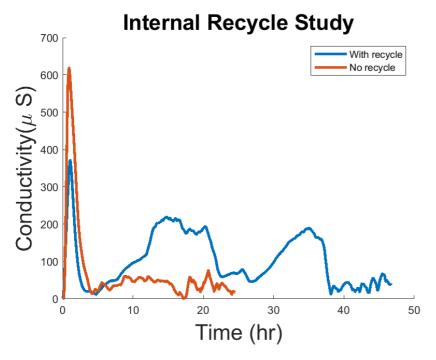


FIGURE 0.8: INTERNAL RECYCLE STUDY

#### 4.3 Internal Recycle Experiment

Figure (4.8) shows the results of the RTD with and without the internal recycle turned on.

The initial peak for both trials are located at the same time but the probability is much lower when there is a recycle. The RTD with respect to time was compared rather than the dimensionless time because the two plots have two different mean residence times. The second and third peaks are not present in the trial without the recycle.

#### 4.4 Characteristic Parameters

#### 4.4.1 Dead-Space and By-passing

The mean residence time for the system without a recycle was found to be 7.02 hrs. This value is compared to the theoretical mean residence time for the reactor of 6.5hrs. As the observed mean residence time is larger than the theoretical, this signifies by-passing in the system. The volumetric flow rate for by-passing was found to be 0.75 L/hr which represents 7.5% of the flow rate in the feed stream.

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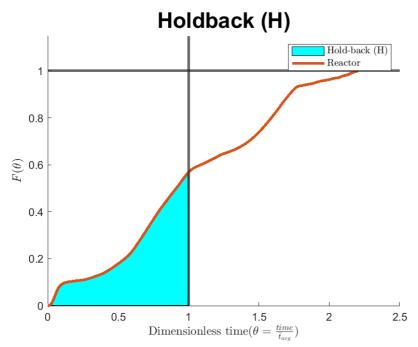


FIGURE 0.9: HOLD-BACK FOR THE VERTICAL BIOREACTOR

#### 4.4.2 Hold-back and Segregation

The plot for the Distribution Function (F(t)) was found with Matlab using the "trapz" function across the Population Density Function (E(t)). The Hold-Back value of H was than obtained from the area under the curve from  $\theta = 0$  to  $\theta = 1$ . This area was found again with the "trapz" function in Matlab (Figure 4.9). The value H was found to be 0.2365.

The value for segregation (S) was found from plotting the F(t) with the F(t) for the ideal CSTR. The intersecting points were found with a Matlab script. Since the plots do not meet at set points, a certain tolerance (< 0.00001) was used to find their intersection. The intersection points than had to be hard coded into the Matlab program. From the plot (Figure 0.10), it may appear that the system exhibits a dead-space with the CSTR proceeding the system.

Your English is very hard to understand !!!!!

Commented [WU168]:

Commented [WU169]: Than is not then. grammar

Commented [WU170]: WHAT SYSTEM ???

Commented [WU171]: Proceeding ????

This is incorrect as there is a small region where the **system** proceeds the CSTR which is difficult to observe due to the scaling of the figure. The zoomed-in Figure 0.11 more clearly shows that the CSTR does in fact **proceed** the reactor. This is evidence that there is no dead-space in the **system**.

SYSTEM, SYSTEM, SYSTEM .....

The value of segregation (S) was found to be -0.16. (Soooo?)

MATLAB IS NO SUBSTITUTE FOR CHEMICAL ENGINEERING IT IS ONLY A SERIES OF ALGORITHMS THAT CAN BE USEFUL. A THESIS MUST BE BASED ON SOLID CHEMICAL ENGINEERING REFER TO MATLAB ONLY IN THE APPENDIX. KNOWLEDGE AND, OFTEN, AN ALGORITHM HIDES THE MEANING OF A PROCESS. COMPUTER TECHNIQUES MUST NOT HIDE CHEMICAL ENGINEERING.

Commented [WU172]: Is this English???

Commented [WU173]: TOO MANY TIMES SYSTEM.

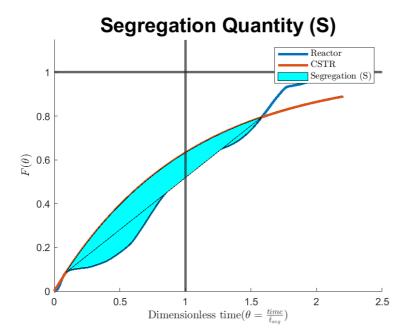


FIGURE 0.10: SEGREGATION (S) FOR THE VERTICAL BIOREACTOR

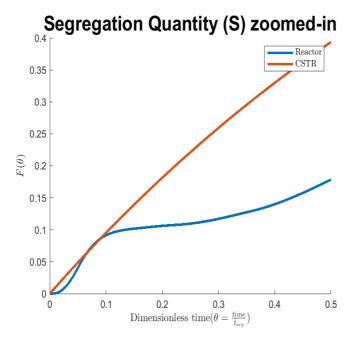


FIGURE 0.11: ZOOMED-IN SEGREGATION (S)

EXPLAIN WHAT IS SEGREGATION, IN THIS CONTEXT, AND HOW THE FLOW AND PERFORMANCE OF THE VERTICAL BIOREACTOR ARE AFFECTED

#### : Discussion CHAPTER number?

The results of the tracer experiment show that the mixing profile of the vertical bioreactor can be obtained. A plot of the Residence Time Distribution (RTD) was obtained and repetition had had shown to be consistent (Figure 4.2). Through analysis of the constructed RTD, different mixing models were evaluated (name them !!!). Table 7 shows that all of the CSTR in series model variants (including generalized Nth and the enhanced), the open and low dispersion models as well as the ideal CSTR accurately fit the mixing profile. It is of note that the dispersion coefficients (0.31 for low and 0.39 for open) are much greater than 0.01 and thus represent a large deviation from Plug Flow[3].

INDICATE THAT THE AXIAL DISPERSION MODEL IS <u>BY DEFINITION</u>, COMPLETELY DIFFERENT FROM THE PF MODEL WITH NO MIXING. SO THE DIFFERENCE IS EXPECTED.

This evidence suggest a high level of mixing in a vertical bioreactor (Indicate the evidence). The ideal CSTR was a very good fit while the ideal PFR was very poor. This is important for two reasons:

- It supports the claim of a high level of mixing due to the reactor geometry[2]
- High levels of mixing are desirable to secure flow uniformity and avoid stagnancies in wastewater treatment bioreactors

Secondary findings show - based on the internal recycle testing - that the reactor exhibits a by-passing of 7.5% of the feed stream. The values for the Hold-back (0.2365) and for Segregation (-0.16) were both found. In both cases, their values were close to the ideal CSTR (H 0.3679 and S = 0 respectively).

All evidence collected suggest a high level of mixing within the vertical bioreactor. It supports the claimed of a high level of mixing due to the tubular geometry. Conventional bioreactors in wastewater engineering exhibit poor mixing profiles and poor conversions (due their reaction kinetics). The field of Biological Nutrient Removal (BNR) research is ever expanding and more research into vertical bioreactors is promising.

Some limitations of this research include the assumption that the reactor with clean water will act the same as wastewater. This is a generally accepted assumption, as the density of activated sludge does not vary much for water. There is also a time constraint to consider as the reactor originally took 230 days for the biomass to get to a steady state[2]. In order to insure that each sensor was adequately submerged, fluid levels were "heldback". These actions will in fact affect the flow dynamics of the system to some small degree. These measures were however necessary to obtain consistent readings.

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**Future** The next step for this research would be the application of the wastewater reaction kinetics (such as the ASM2D mentioned in the literature review) across the developed model. These models still require **chemical and microbial** kinetic parameters, which can be found in literature, but due to the complicated nature of a mixed population of microbes would be best found experimentally. This experiment can be performed by seeding the reactor with microbes and developing the population. Samples from each section would be taken and their reaction kinetics found in a batch reactor.

There could be some value in modeling the vertical bioreactor with a Computational Fluid Dynamics (CFD). CFDs can identify the physical locations of dead-space and by-pass within the reactor. There was found to be 7.5% by-passing in the reactor which could be better identified with a CFD. A potential source of by-passing was observed in the anoxic zone 2 Figure 5.1 which was not addressed due to <a href="mailto:current\_public health and hence">current\_public health and hence</a> time restraints. Addressing this concern <a href="mailto:thence">than</a> determining the new amount of by-passing would be an easier solution.

A The-vertical bioreactor has been tested experimentally and shown to be well represented by a CSTR. There is some potential value of using more complicated models to represent the mixing profile such as the Axial Dispersion model or the Generalized N-CSTR in series model. They both require only one parameter but the Axial Dispersion model may give some the impression that the system is similar to the PFR. As expected, It is important to remember that the Dispersion coefficient D in this study is very high high (Hence the approximation to a CSTR) and which-represents a large deviation RELATIVE for the ideal PFR. The system also exhibits a by-passing of 7.5%

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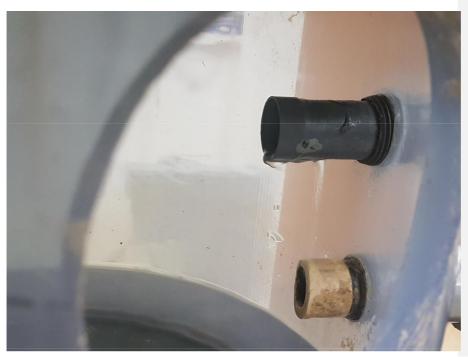


FIGURE 0.1: POTENTIAL SOURCE OF BY-PASSING

What is this ????

## : Conclusions, section number???

The mixing profile for a vertical bioreactor was found by performing a tracer experiments. A tracer solution of 50mL saturated NaCl was injected at the entrance of the reactor and the conductivity was measured at the exit of each stage. The collected data was then converted into the dimensionless Residence Time Distribution (RTD). The behaviour of the flow was interpreted from these results with the effect of the internal recycle evident. There was no evidence of dead-space but 7.5% by-passing was found.

The mixing profile was than compared to both ideal and real reactor models. It was found that the generalized Nth CSTR in series model and the Ideal CSTR fit the mixing profile observed in the vertical bioreactorwell. The parameters for Hold-back (H) and Segregation (S) were found to be 0.2365 and -0.16 respectively. In both cases, this suggest a high level of mixing similar to the ideal CSTR behaviour.

THE CONCLUSIONS IN POINT FORM and chapter number

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# Appendix

PLACE IN YOUR APPENDIX : WELL KNOWN CHEMICAL ENGINEERING MATERIAL.

### Bibliography

# CHECK CAREFULLY ALL YOUR REFERENCES AND STUDY <u>ALL</u> THE PUBLICATIONS BY REZA AND ALVAREZ CUENCA

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