

# QUANTITATIVE FR 13 FAILURE MODELLING OF UV IRRADIATION FOR POTABLE WATER PRODUCTION – DEMONSTRATED WITH ESCHERICHIA COLI

by

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Dedicated especially to

My dear parents, Abdul Halim Mansor & Ezizah Hashim

My lovely husband, Ahmad Spahirulfitri Kabibi Mohd Rudin

> My precious sons, Adel Rayyan & Aleef Daniel

And in loving memory of my brave nephew who passed away too young, too soon at the age of five (5) after fighting a brave battle with brain tumor for three (3) years.

Srsyad Hakimi Ahmad Fadzly Effendy (1 December 2010 - 7 August 2016)

"Acquire knowledge, and learn tranquility and dignity"

Umar ibn Al-Khattab

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## PREFACE

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### **EXECUTIVE SUMMARY**

Steady-state ultraviolet (UV) irradiation for potable water production is becoming an important global alternative to traditional disinfection by chlorination. Failure of UV to reduce the number of viable contaminant pathogens however can lead to enduring health legacies (with or without fatalities).

To better understand vulnerability of UV operations to failure, the probabilistic *Fr 13* risk framework of Davey and co-workers<sup>1</sup> is applied for the first time in this thesis. *Fr 13* is predicated on underlying chemical engineering unit-operations. It is based on the hypothesis that naturally occurring, chance (stochastic) fluctuations about the value of 'set' process parameters can unexpectedly combine and accumulate in one direction and leverage significant change across a binary 'failure– not failure' boundary. Process failures can result from the accumulation of these fluctuations within an apparent steady-state process itself. That is to say, even with good design and operation of plant, there can be unexpected (surprise and sudden) occasional failures without 'human error' or 'faulty fittings'.

Importantly, the impact of these naturally occurring random fluctuations is not accounted for explicitly in traditional chemical engineering.

Here, the Fr 13 risk framework is applied for the first time to quantitatively assess operations of logically increasing complexity, namely, a laminar flow-through UV reactor, with turbulent flow in a concentric annular-reactor, both with and without suspended solids

<sup>&</sup>lt;sup>1</sup> Davey, K.R., Chandrakash, S. & O'Neill, B.K. 2015. A Friday 13<sup>th</sup> failure assessment of clean-in-place removal of whey protein deposits from metal surfaces with auto-set cleaning times. *Chemical Engineering Science* **126**, 106-115. <u>http://dx.doi.org/10.1016/j.ces.2014.12.013</u>

Zou, W. & Davey, K.R. 2016. An integrated two-step *Fr 13* synthesis – demonstrated with membrane fouling in combined ultrafiltration-osmotic distillation (UF-OD) for concentrated juice. *Chemical Engineering Science* 152, 213-226. <u>http://dx.doi.org/10.1016/j.ces.2016.06.020</u>

present (Davey, Abdul-Halim and Lewis, 2012; Davey and Abdul-Halim, 2013; Abdul-Halim and Davey, 2015; 2016)<sup>2</sup>, and; a two-step 'global' risk model of combined rapid-sand-filtration and UV irradiation (SF-UV) (Abdul-Halim and Davey, 2017)<sup>3</sup>. The work is illustrated with extensive independent data for the survival of viable *Escherichia coli* - a pathogenic species of faecal bacteria widely used as an indicator for health risk.

A logical and step-wise approach was implemented as a research strategy.

UV reactor unit-operations models are first synthesized and developed. A failure factor is defined in terms of the design reduction and actual reduction in viable *E. coli* contaminants. UV reactor operation is simulated using a refined Monte Carlo (with Latin Hypercube) sampling of UV lamp intensity (*I*), suspended solids concentrations [*conc*] and water flow (*Q*). A preliminary *Fr 13* failure simulation of a single UV reactor unit-operation (one-step), developed for both simplified laminar flow and turbulent flow models, showed vulnerability to failure with unwanted survival of *E. coli* of, respectively, 0.4 % and 16 %, averaged over the long term, of all apparently successful steady-state continuous operations. A practical tolerance, as a design margin of safety, of 10 % was assumed. Results from applied 'second-tier' studies to assess re-design to improve UV operation reliability and safety and to reduce vulnerability to *Fr 13* failure showed that any

<sup>&</sup>lt;sup>2</sup> Abdul-Halim, N. & Davey, K.R. 2016. Impact of suspended solids on *Fr 13* failure of UV irradiation for inactivation of *Escherichia coli* in potable water production with turbulent flow in an annular reactor. *Chemical Engineering Science* 143, 55-62. <u>http://dx.doi.org/10.1016/j.ces.2015.12.017</u>

Abdul-Halim, N. & Davey, K.R. 2015. A Friday 13th risk assessment of failure of ultraviolet irradiation for potable water in turbulent flow. *Food Control* 50, 770-777. http://dx.doi.org/10.1016/j.foodcont.2014.10.036

Davey, K.R. & Abdul-Halim, N. 2013. Friday 13<sup>th</sup> risk modelling: A new risk model of UV irradiation for potable water. In: Proc. International Association for Food Protection, European Symposium on Food Safety – IAFP 2013, Marseille, France, May 15-17. http://www.foodprotection.org/europeansymposium/2013/

Davey, K.R., Abdul-Halim, N. & Lewis, D. 2012. Friday 13<sup>th</sup> failure modelling: a new quantitative risk assessment of UV irradiation for potable water. In: Proc. 42<sup>nd</sup> Australasian Chemical Engineering Conference (Quality of Life through Chemical Engineering) - CHEMECA 2012, Wellington, New Zealand, September 23-26, paper 92. ISBN 9781922107596

<sup>&</sup>lt;sup>3</sup> Abdul-Halim, N. & Davey, K.R. 2017. A microbial risk model for *Escherichia coli* in sequential rapid sand-filtration and ultraviolet irradiation in an annular reactor for potable water. *Chemical Engineering Science – in preparation* (March).

increased costs to improve control and reduce fluctuations in raw feed-water flow, together with reductions in UV lamp fluence, would be readily justified. The *Fr 13* analysis was shown to be an advance on alternate risk assessments because it produced all possible practical UV outcomes, including failures.

A more developed and practically realistic model for UV irradiation for potable water production was then synthesized to investigate the impact of the presence of suspended solids (SS) (median particle size 23 µm) as UV shielding and UV absorbing agents, on overall UV efficacy. This resulted in, respectively, some 32.1 % and 43.7 %, of apparent successful operations could unexpectedly fail over the long term due, respectively, to combined impact of random fluctuations in feed-water flow (Q), lamp intensity  $(I_0)$  and shielding and absorption of UV by SS [conc]. This translated to four (4) failures each calendar month (the comparison rate without suspended solids was two (2) failures per month). Results highlighted that the efficacy of UV irradiation decreased with the presence of SS to 1-log<sub>10</sub> reduction, compared with a 4.35-log<sub>10</sub> reduction without solids present in the raw feed-water. An unexpected outcome was that UV failure is highly significantly dependent on naturally occurring fluctuations in the raw feed-water flow, and not on fluctuations in the concentration of solids in the feed-water. It was found that the initial presence of solids significantly reduced the practically achievable reductions in viable bacterial contaminants in the annular reactor, but that fluctuations in concentration of solids in the feed-water did not meaningfully impact overall vulnerability of UV efficacy. This finding pointed to a pre-treatment that would be necessary to remove suspended solids prior to the UV reactor, and; the necessity to improve control in feedwater flow to reduce fluctuations.

The original synthesis was extended therefore for the first time to include a rapid sand-filter (SF) for pre-treatment of the raw feed-water flow to the UV reactor, and; a

ix

*Fr 13* risk assessment on both the SF, and sequential, integrated rapid sand-filtration and UV reactor (SF-UV). For the global two-step SF-UV results showed vulnerability to failure of some 40.4 % in overall operations over the long term with a safety margin (tolerance) of 10 %. Pre-treatment with SF removed SS with a mean of 1-log<sub>10</sub> reduction (90 %). Subsequently, an overall removal of viable *E. coli* from the integrated SF-UV reactor was a 3-log<sub>10</sub> reduction (99.9 %). This is because the efficacy of UV light to penetrate and inactivate viable *E. coli*, and other pathogens, is not inhibited by SS in the UV reactor. This showed that the physical removal of *E. coli* was accomplished by a properly functioning SF and subsequently disinfection was done by UV irradiation to inactivate viable *E. coli* in the water.

Because the Regulatory standard for potable water is a 4-log<sub>10</sub> reduction, it was concluded that flocculation and sedimentation prior to SF was needed to exploit these findings. Flocculation is a mixing process to increase particle size from submicroscopic microfloc to visible suspended particles prior to sedimentation and SF.

This research will aid understanding of factors that contribute to UV failure and increase confidence in UV operations. It is original, and not incremental, work.

Findings will be of immediate interest to risk analysts, water processors and designers of UV reactors for potable water production.

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## TABLE OF CONTENTS

PAGE

Declara	tion	iii
Preface		v
Executiv	ve Summary	vii
Acknow	ledgments	xi
Table of	Contents	xiii
List of <b>T</b>	. ables	xvii
List of F	ìigures	xix
Chapter	1: Introduction	1
1.1	Background	2
1.2	Research aims	3
1.3	Justification for the research	4
1.4	This thesis	4
Refe	rences	6
Chapter	2: Literature Review	9
2.1.	Introduction	10
	2.1.1. Traditional single value assessment (SVA) solutions	12
2.2.	Friday 13th failure	13
	2.2.1. <i>Fr 13</i> failure modelling	13
	2.2.2. <i>Fr 13</i> and other risk approaches	16
	2.2.3. <i>Fr 13</i> as terminology	18
	2.2.4. Chance and uncertainty	18
	2.2.5. Application of Fr 13 risk assessment	19
	2.2.6. Advantages and limitations of Fr 13	23
	2.2.7. Fr 13 risk assessment for UV irradiation unit-operation	25
2.3.	Ultraviolet irradiation	26
	2.3.1. UV light	25
	2.3.2. Mechanism of UV irradiation	28
	2.3.3. UV irradiation for potable water production	29
	2.3.4. Advantages and disadvantages of UV irradiation for potable water	31
	2.3.5. UV reactors configuration	33
2.4.	Shortcomings	35
2.5	Summary and conclusions	36
Refe	rences	38
Chapter	<sup>9</sup> 3: Friday 13 <sup>th</sup> Failure Modelling: A New Quantitative Risk Assessmen	nt
•	of UV Irradiation for Potable Water	50
State	ment of Authorship	52
Abst	Abstract	

3.1.	Introduction	55
3.2.	A model for UV irradiation	56
3.3.	Fr 13 failure model	58
	3.3.1. Defining UV Failure	58
	3.3.2. Simulating <i>Fr</i> 13	58
3.4.	Results	60
3.5.	Discussion	61
3.6.	Conclusions	62
Nota	ation	64
Refe	References	

Chapter	: 4: <i>Fr 13</i> Failure Modelling of UV Irradiation with Turbulent Flo	ow in
	an Annular Reactor	69
State	ement of Authorship	71
Abst	ract	73
4.1.	Introduction	75
	4.1.1. This study	77
4.2.	Materials and Methods	78
	4.2.1. The annular UV reactor of Ye (2007)	78
	4.2.2. Traditional single point simulation	82
4.3.	Fr 13 simulation	83
	4.3.1. Defining UV failure	83
	4.3.2. r-MC sampling	84
	4.3.3. <i>Fr 13</i> model	84
4.4.	Results	85
4.5.	Discussion	88
	4.5.1. <i>Fr 13</i> failures	88
	4.5.2. Visualizing <i>Fr 13</i> risk	89
	4.5.3. Input probability distributions for <i>Fr 13</i>	91
	4.5.4. Minimizing Fr 13 risk	93
	4.5.5. Turbulent vs laminar flow Fr 13 failures	96
	4.5.6. Coupling <i>Fr 13</i> with commercial technologies	97
4.6.	Conclusions	98
Nom	enclature	99
Refe	References	

Chapter 5: Impact of Suspended Solids Concentration on Fr 13 Failure of UV	
Irradiation for Potable Water in Turbulent Flow	105
Statement of Authorship	107
Abstract	109
5.1. Introduction	111
5.1.1. Purpose of this study	113
5.2. Materials and methods	114
5.2.1. UV inactivation of <i>E. coli</i> with suspended solids present	114

	5.2.2.	An annular UV reactor unit-operations with turbulent flow	116
	5.2.3.	Traditional single value assessment (SVA) simulation	118
	5.2.4.	Fr 13 model and simulation	119
5.3.	Result	S	121
5.4.	Discus	ssion	125
	5.4.1.	Model confirmation	125
	5.4.2.	Ability to identify each Fr 13 event	126
	5.4.3.	Impact of suspended solids	126
	5.4.4.	UV lamp intensity and dose	130
	5.4.5.	Results overview	131
5.5.	Conclu	isions	133
Nomenclature		135	
References		137	

### Chapter 6: A Global Microbial Risk Model for *Escherichia Coli* in Two-Step Sand-Filtration and Ultraviolet Irradiation (SF-UV) for Potable Water

	in an Annular Reactor	145
State	Statement of Authorship	
Abs	tract	149
6.1.	Introduction	151
	6.1.1. Purpose of this study	153
6.2.	Materials and methods	154
	6.2.1. Rapid sand-filter (SF)	155
	6.2.2. UV inactivation of viable <i>E. coli</i>	158
	6.2.3. Concentric annular UV reactor	159
	6.2.4. SF-UV global model	161
6.3.	Traditional, deterministic Single Value Assessment (SVA)	161
6.4.	Fr 13 model simulations	164
	6.4.1. Failure factors	164
	6.4.2. Fr 13 simulations	165
6.5.	Results	166
6.6.	Discussion	172
	6.6.1. SF-UV global model	172
	6.6.2. Presentation of risk results	177
	6.6.3. Efficacy of integrated SF-UV	178
	6.6.4. <i>Fr 13</i> and second-tier simulations	179
	6.6.5. Improving integrated SF-UV	181
6.7.	Conclusions	181
Non	nenclature	183
Refe	erences	186
Chapte	r 7: Conclusions	191
7.1	Conclusions	192
7.2	Future development	196

**APPENDIX A** – A Definition of Some Important Terms Used in This Research198**APPENDIX B** – Friday 13<sup>th</sup> Failure Modelling: A New Quantitative Risk Assessment200**APPENDIX C** – A Friday 13th Risk Assessment of Failure of Ultraviolet Irradiation for<br/>Potable Water in Turbulent Flow209**APPENDIX D** – Friday 13th Risk Modelling: A New Risk Model of UV Irradiation for

Potable Water 218

APPENDIX E – Impact of Suspended Solids on *Fr 13* Failure of UV Irradiation for Inactivation of *Escherichia coli* in Potable Water Production with Turbulent Flow in an Annular Reactor 220

## LIST OF TABLES

## PAGE

Table 2.1 Table 2.2	Summary and chronological listing of <i>Fr 13</i> risk assessments Summary of UV spectrum range	20 28
Table 2.2     Table 2.3	Advantages and disadvantages of UV irradiation for potable water production as an alternative to chlorination method	32
Table 3.1	Comparison of traditional single point (SVA) and $Fr 13$ risk assessments for UV irradiation for potable water with the Davey Linear Arrhenius equation for inactivation of $F_{r}$ coli	60
Tabla 3.7	5 failures from 47 in 10 000 LIV irradiation scenarios	61
Table J.2 Table / 1	Comparison of traditional single point (SVA) and Er 13 risk	86
1 aute 4.1	assessments for turbulent flow in 4-series annular-reactor	80
Table 4.2	Twenty (25) selected failures from 1,604 in 10,000 UV irradiation scenarios	87
Table 4.3	Comparison of Model I (laminar flow reactor of Davey and co-	96
	workers (2012)) with <b>Model II</b> (turbulent flow annular-reactor of Ye (2007) and Ye and co-workers (2008)) for UV irradiation of <i>E. coli</i> for potable water	
Table 5.1	Coefficients for the Davey linear-Arrhenius (DL-A) model for UV irradiation inactivation of viable <i>E. coli</i> in the presence of suspended solids as both UV shielding and UV absorbing agents	115
	$\ln k = C_0 + C_1 [dose] + C_2 [dose]^2 + C_3 [conc]$	
	with k in $\mu W^{-1} s^{-1} cm^2$ for a range of concentration of shielding agent	
	$0.01 \le [conc] \le 0.3$ , g L <sup>-1</sup> and absorbing agent $0.001 \le [conc] \le 0.03$ , g L <sup>-1</sup>	
Table 5.2	Comparison of traditional SVA with <i>Fr 13</i> assessment for UV irradiation inactivation of viable <i>E. coli</i> with DL-A kinetics in the presence of UV shielding agent with a % <i>tolerance</i> = 10 % in turbulent flow in the annular reactor	122
Table 5.3	Twenty (20) selected failures from 3,205 in 10,000 UV irradiation scenarios for UV shielding agent	124
Table 5.4	Spearman rank correlation coefficient (Snedecor and Cochran, 1989) for the three key input parameters of the annular reactor on UV risk factor $(p)$	129
Table 6.1	Coefficients for the Davey linear-Arrhenius (DL-A) model for UV irradiation inactivation of viable <i>E. coli</i> (ATCC 25922 'Seattle' strain) in the presence of suspended solids as UV shielding agent (Amos et al., 2001) in which $\ln k = C_0 + C_0 [dose]^2 + C_0 [conc]_{cm}$	159
	with k in $\mu$ W <sup>-1</sup> s <sup>-1</sup> cm <sup>2</sup> for a range of concentration of shielding agent 0.01 $\leq$ [conc] $\leq$ 0.3, g L <sup>-1</sup>	1.00
Table 6.2	Traditional single value assessment (SVA) for global SF-UV	163

	inactivation of <i>E. coli</i> in feed-water flow.	
Table 6.3	Comparison of traditional SVA with Fr 13 risk assessment for	167
	particle removal in rapid sand-filtration (SF) with a % tolerance	
	(safety margin) = 10 %	
Table 6.4	Ten (10) selected Fr 13 failures from 2,000 in 10,000 scenarios for	170
	SS removal in SF with a 10 % tolerance. (The <b>bolded text</b> of column	
	5, failure 4, is the particular scenario shown in Table 6.3)	
Table 6.5	Corresponding output scenarios for UV reactor with the 10 failures in	171
	SF of Table 6.4 as inputs with 10 % tolerance. (The <b>bolded text</b> of	
	column 5, failure 4, is the particular scenario shown in Table 6.3)	
Table 6.6	Ten (10) selected Fr 13 scenarios of the global SF-UV demonstrated	174
	with E. coli	
Table 6.7	Visual summary of the 10 selected Fr 13 scenarios of Table 6.6 for	175
	the combined SF-UV global model demonstrated with E. coli with a	
	10 % tolerance	
Table 6.8	Spearman rank correlation coefficient (Snedecor and Cochran, 1989)	177
	for the key input parameters on risk factor $(p_2)$ in the global SF-UV	
	model	

## LIST OF FIGURES

Fig. 2.1	The 5-step algorithm of the <i>Fr 13</i> framework pioneered by The University of Adelaide researchers of the emerging new analytical tool for quantitative process safety	14
Fig. 2.2	UV spectrum (Adapted from Anon., 2006)	27
Fig. 2.3	Schematic diagram of an open-channel UV irradiation with (a) vertical lamp configuration (b) horizontal lamp configuration (Adapted from Ye, 2007)	34
Fig. 2.4	Schematic diagram of a thin film annular-reactor between two concentric cylinders (Adapted from Ye, 2007).	35
Fig. 4.1	Schematic diagram of a thin film annular-reactor between two concentric cylinders (Adapted from Ye, 2007).	78
Fig. 4.2	The 4-series annular-reactor of Ye (Adapted from Ye et al., 2008)	81
Fig. 4.3	Distribution for the risk factor ( <i>p</i> ) for UV irradiation for potable water in turbulent flow in the 4-series annular-reactor	87
Fig. 4.4	Plot of the 25 selected <i>Fr 13</i> failures ( $p > 0$ ) of Table 4.2: 3D scatter plot (a) and 3D surface plot (b)	90
Fig. 4.5	Effect of <i>%tolerance</i> on $log_{10}$ reduction in viable <i>E. coli</i> against the number of <i>Fr 13</i> failures per 10,000 scenarios of continuous UV irradiation for potable water in the 4-series annular-reactor	94
Fig. 4.6	Effect of variability (%-stdev) on the volumetric flow rate ( $Q = 180$ mL s <sup>-1</sup> ) against the number of <i>Fr 13</i> failures in UV irradiation for	95
Fig. 5.1	Distribution for the risk factor ( <i>p</i> ) from 10,000 scenarios of UV irradiation for inactivation of viable <i>E. coli</i> in the presence of UV shielding agent in turbulent flow in the annular reactor. Failure is defined for all $n > 0$	124
Fig. 5.2	Impact of %-stdev in distributions for combined, suspended solids as UV shielding agent [ <i>conc</i> ], feed water flow ( <i>Q</i> ) and lamp intensity ( $I_0$ ), on the number of <i>Fr 13</i> failures per 10,000 scenarios in UV irradiation of viable <i>E. coli</i> for potable water with DL-A inactivation kinetics in turbulent flow in the annular reactor	128
Fig. 5.3	Impact of UV dose on reduction of numbers of viable <i>E. coli</i> , with DL-A inactivation kinetics, in the presence of UV shielding agent, $[conc] = 0.115 \text{ g L}^{-1}$ , in turbulent flow in the annular reactor	130
Fig. 6.1	Schematic of conventional treatment for potable water production. Highlighted is the integrated SF-UV unit-operations	155
Fig. 6.2	Rapid sand-filtration (SF) for SS removal	156
Fig. 6.3	Distribution for the risk factor ( $p_1$ ) from 10,000 scenarios of rapid sand-filtration (SF). All $p_1 > 0$ highlight a failure	168

Distribution for the risk factor $(p_2)$ from 10,000 scenarios of the	176
sequential SF-UV operations, where $p_2 > 0$ is a failure	
Impact of %tolerance on the number of overall integrated SF-UV	180
failures $(p_2)$ per 10,000 scenarios	
Multi-step unit-operation processes in potable water production.	197
Highlighted is the future work that can be developed for Fr 13 risk	
framework	
	Distribution for the risk factor $(p_2)$ from 10,000 scenarios of the sequential SF-UV operations, where $p_2 > 0$ is a failure Impact of <i>%tolerance</i> on the number of overall integrated SF-UV failures $(p_2)$ per 10,000 scenarios Multi-step unit-operation processes in potable water production. Highlighted is the future work that can be developed for <i>Fr 13</i> risk framework

## **CHAPTER ONE**

**INTRODUCTION** 

#### 1.1. Background

Water is essential for all living things. According to the World Health Organization (Anon., 2001), inadequate drinking water and poor quality sanitation are one of the world's major causes of, particularly, human death (Anon., 2001). Potable water is therefore a very important determinant for human health, and; consequently treatments to produce potable water have been variously developed. One of the most widely used is ultraviolet (UV) irradiation applied as a unit-operation (*see* for e.g. Elyasi, 2009; Bolton, 2000; Cassano et al., 1995; Severin et al., 1984; Nguyen, 1999; Amos et al., 2001; Brahmi et al., 2010).

However failure of UV plant with unwanted survival of viable pathogens can lead to an enduring public health legacy, with or without fatalities. An understanding of risk and ways to reduce vulnerability to failure for UV production of potable water is therefore globally important.

Of emerging research interest is the practical notion that no matter how good the design and operation of a process unit-operation, there will be an occasional, unexpected (surprise) failure. Often "human error" or "faulty fittings" is blamed for the failure. However, an original hypothesis of Davey and co-workers (The University of Adelaide) is that failure of plant and product can result from accumulation of naturally occurring, random (stochastic) fluctuations in key parameters that unexpectedly combine in one direction to leverage change in plant outcome behaviour. Failure of otherwise well-operated, well-maintained processes has been titled *Friday 13<sup>th</sup> failure (Fr 13)* - to indicate the surprise nature of the event (e.g. Davey, 2011; 2010; Langer, 2008; Cerf and Davey, 2001; Abdul-Halim and Davey, 2015; 2016; Patil et al., 2005; Chandrakash et al., 2015; Zou and Davey, 2016). Major advantages of the *Fr 13* framework include that it is highly quantitative, provides new insight into plant behviour outcomes not availabe from

alternative risk methodologies, and; is based on established unit-operations principles in chemical engineering (Foust et al., 1980).

Despite the global importance of UV irradiation for potable water and the need for a safe water supply, its vulnerability to failure as a process unit-operation has not been investigated. Against this background a research study of the risk and vulnerability to failure of continuous UV irradiation for potable water was carried out using the Fr 13 risk framework and methodology.

#### 1.2. Research aims

The overall aim of this research is to explore for the first time a quantitative *Fr 13* assessment of the risk of failure in an otherwise well-operated and well-maintained unitoperation of UV irradiation for potable water production and compare this with traditional risk methods. UV failure is defined as a level of unwanted survival of a contaminant, viable pathogen.

Specific research aims are to:

- 1. Determine quantitatively the vulnerability to unexpected failure of UV irradiation
- 2. Determine process parameters that most significantly influence Fr 13 failures
- To gain new insights initially into failure of single-step UV process and to gradually develop and investigate a 2-steps UV process subsequent to sandfiltration process
- Assess the impact of possible targeted intervention strategies designed to minimize risk of *Fr 13* failure in UV irradiation for potable water production, and to improve process safety.

Operating conditions will be chosen with a view to applying findings to realistic problems related to the large-scale UV irradiation for potable water production.

#### **1.3.** Justification for the research

This research is readily justified because it will lead to greater understanding of the factors that contribute to vulnerability to failure of primarily UV irradiation in a single-step process and the two-step sand-filtration and UV process, for potable water production. An increased understanding of Fr 13 risk will lead to increased confidence in the design and performance of UV irradiation plant and the likely success of proposed intervention strategies. Results are also more generalized and widely applied.

By combining research findings with established work it is hoped to exploit this new research technology for community benefit through safeguarding UV irradiation for potable water and to advance design excellence through a new understanding of process risk.

#### 1.4. This thesis

A logical and step-wise approach to the research is adopted.

The relevant literature is reviewed in Chapter 2 and the advantages of using UV irradiation for potable water production are examined. The importance of notions of uncertainty and variability in risk assessments are highlighted and the shortcomings of current risk assessment approaches are discussed.

In Chapter 3, a Fr 13 risk assessment is synthesised for the first time for a simplified, laminar-flow model for UV irradiation for potable water production. A comparison is made between the predictions from the new Fr 13 model and traditional

(bio) chemical engineering approaches. A UV process risk factor (p) is defined and a refined Monte Carlo (r-MC) simulation (with Latin Hypercube) sampling used for simulations. The model is demonstrated with independent data for *Escherichia coli* – a pathogenic species of bacteria widely used as an indicator of health risk. Practical methods to reduce vulnerability to surprise failure and improve UV process technology for potable water are illustrated.

In Chapter 4, *Fr 13* risk assessment is investigated as a more developed unit-operation for UV irradiation for potable water in turbulent flow in a series annularreactor. This chapter demonstrates the effects of stochastic (random) changes in UV parameters on plant failure. Refined Monte Carlo (r-MC) with Latin Hypercube sampling is again illustrated. The work is shown to be a significant advance on current risk assessments because it produces all possible practical UV plant outcome behaviour.

In Chapter 5, the probabilistic Fr 13 failure model is further developed to include the impact of suspended solids on UV efficacy for the first time. This chapter concludes with practical recommendations to improve UV efficacy and reduce failure risk with raw feed water with suspended solids concentrations.

In Chapter 6, the UV *Fr* 13 failure model is combined with sequential rapid sandfiltration (SF) to pre-filter the raw feed water. This notion of a *Fr* 13 global model for potable water production is discussed.

The overall findings of this research are summarised in Chapter 7.

Some important terms used in this research work are defined in Appendix A.

A list of refereed publications arising from this research is presented in Appendices B, C, D and E.

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## CHAPTER TWO

## LITERATURE REVIEW

#### 2.1. Introduction

The definition of process risk is actually relatively new - and developing. At present there is no universally adopted definition (Yoe, 2012; Covello and Merkhoher, 1993). Risk and risk assessment therefore have a range of definitions (which can sometimes be confusing). This is because most risk assessments have been developed specifically to address risk in particular disciplines. The US Environmental Protection Agency (USEPA), for example, identifies 18 variations on the meaning of risk (Yoe, 2012).

In the microbiological literature *Microbiological risk assessment* is widely used and is defined in the Codex Alimentarius (CAC, 1998). However it is considered ambiguous because of a lack of 'process'- and because 'risk' is sometimes reported when what is actually meant is 'hazard' (Davey, 2010; Whiting and Buchanan, 1997; Thomas et al., 2006).

A widely adopted risk assessment in the foods industries is *Hazard Analysis Critical Control Point (HACCP). HACCP* is a preventive approach for quality control. It systematically looks at physical, chemical, and biological hazards as a means of prevention - rather than an inspection of finished product (Mortimore and Wallace, 1994). A drawback is there is no defined method, or template, as to how a process plant should be inspected. As a result, findings are often semi-quantitative only (Davey, 2010).

In the engineering literature *Hazard and Operability* (*HAZOP*) studies are well established. *HAZOP* is used to determine problems by exploring the impact of any deviations from design conditions. *HAZOP* is a highly disciplined procedure but it suffers from the fact that it is a qualitative technique based on guide-words. *Reliability* 

10

*Engineering* is also widely used - but is restricted to expected failure without catastrophic consequences (O<sup>2</sup>Connor et al., 2002).

In recent years risk programs have been established in both Australia and France for e.g. *The Australian Centre of Excellence for Risk Analysis*, in the School of Botany, The University of Melbourne (established 2006) and *Met@risk: Methods for Food Risk Analysis*, l'Institut National de la Recherche Agronomique, Paris (created 2004). However, the research does not focus on chemical engineering unit-operations or whole-of-process but rather, is limited to 'hazards' for, respectively, 'import clearance', 'response actions for invasive species' and 'decision making in complex systems', and; 'human dietary exposure' and 'socio-economic analyses of regulatory measures' (Davey, 2010).

Some major problems in risk research programs include (Zou, 2015):

- i. Understandable confusion regarding terminology in the literature
- ii. What exactly is going to be done
- iii. Whether findings are qualitative or quantitative in nature
- iv. How results will be reported.

Practically, many publications titled 'risk assessment' do not provide quantitative insight into unanticipated and often catastrophic process plant failure. This is one reason why, 'human error' or 'faulty fittings' are widely blamed for unanticipated failure (Cerf and Davey, 2001; Langer, 2008).

For this research, risk is defined as the probability that an adverse effect will occur (Notermans and Mead, 1996; Vose, 2008). This is defined as the probability of failure for UV irradiation with presence of the viable pathogen *Escherichia coli* in the treated water.

In this chapter, a review of the Fr 13 framework is presented and discussed in detail. Recent developments, applications, benefits and limitations are presented and a

comparison is made with traditional unit-operations solutions and alternative risk techniques.

UV irradiation for potable water production was chosen for this study to test and advance the Fr 13 framework. This is timely as UV irradiation has been widely adopted in water treatment as an alternative to disinfection with chlorination.

The properties of UV irradiation and failure mechanisms of UV irradiation unitoperations models are identified and evaluated.

To conclude this chapter, a concentric annular UV reactor was selected to illustrate to test the Fr 13 framework.

2.1.1. Traditional single value assessment (SVA) solutions

The traditional method to computationally solve foods and chemicals engineering unit-operations is a single point, deterministic approach, with or without a sensitivity analysis (Sinnott, 2005). Cerf and Davey (2001) and Davey and Cerf (2003) defined this methodology as Single Value Assessment (SVA).

In this traditional approach, model inputs are linked together with outputs via mathematical expressions such as multiplication, subtraction, addition and exponentiation. The equations can be conveniently solved in mathematical software e.g. Microsoft Excel<sup>TM</sup> spread sheeting.

A single or 'best estimate' value of input parameters is used to solve for a single 'best estimate' outcome. A variation ( $\pm$  1 to 5, %) is used around the mean value of inputs to test the robustness of model results, for *uncertainty* in process parameters. Almost all chemical unit-operations used in food and bio-processing can be addressed with this method (Foust et al., 1980; McCabe et al., 2001). However, naturally occurring random fluctuations on inputs and their possible impact(s) on plant outcome behaviour are not accounted for explicitly in traditional chemical engineering.

### 2.2. *Friday 13<sup>th</sup>* failure

The notion of Friday  $13^{\text{th}}$  (*Fr 13*) is rooted in history and is perceived as a day of 'bad' luck. It is a notion that has long persisted in the industrial West - and has been observed time and again in a number of variants in plant operations (Suddath, 2009).

The *Fr 13* risk framework has its genesis in the proposal of Davey and Cerf (2003) to explain reoccurring and unexpected (surprise) failures in otherwise well-operated and well-regulated UHT milk processing (Cerf and Davey, 2001; Davey, 2011).

Their hypothesis was that despite good design, operation and maintenance of a plant, there will be an occasional unexpected (sudden) 'bad' outcome. This may result in potential catastrophic or enduring effect to public health, and the economy, with or without fatality. The unexpected failure is often put down to 'human error' or 'faulty or leaky fittings', following, usually, exhaustive official hearings. This, of course, is actually an assertion in need of an explanation (Cerf and Davey, 2001). Surprise failures create loss of faith in manufacturing.

#### 2.2.1. Fr 13 failure modelling

 $Fr \ 13$  risk modeling is an emerging, quantitative process to estimate the likelihood of inherent 'real' risk of failure of process or product. A key insight of this emerging technology is to show that an accumulation and combination of a series of indiscernible,

but practically realizable, changes in otherwise well-operated plant parameters can lead unexpectedly in one-direction and leverage highly significant and catastrophic changes in process or product (Davey and Cerf, 2003).

The framework of *Fr 13* risk assessment is similar to that of the traditional SVA because all mathematical operations (i.e. multiplications, additions, exponentiations, etc) that connected the model parameters are the same (Davey et al., 2015; Chandrakash et al., 2015; Zou and Davey, 2016), except that probability distribution is used instead of the single 'best' guess to define the key input parameters.

 $Fr \ 13$  methodology is based on the 5-step algorithm pioneered by The University of Adelaide researchers. The steps are shown in Fig. 2.1:



**Fig. 2.1:** The 5-step algorithm of the *Fr 13* methodology pioneered by The University of Adelaide researchers of the emerging new analytical tool for quantitative process safety.

The first step for *Fr 13* risk assessment is to identify UV irradiation as an identifiable unit-operation. Usually this is achieved through synthesis and validation of key process parameters in a computational model and software for particular plant throughputs (Zou, 2015). Generally, the criteria for unit-operation model is: accuracy of prediction against observed data; ease of synthesis and use; relative complexity i.e. economy/elegance, a form that can be readily married within an overall process model, and; generalized form applicable to wide range of micro-organism (Amos et al., 2001; Davey et al., 2012).

The second step is to identify the key UV irradiation parameters on failure(s) using traditional engineering, Single Value Assessments (SVA) (Davey and Cerf, 2003; Patil et al., 2005; Davey et al., 2013; Abdul-Halim and Davey, 2016).

The third step is to define parameter values with a probability distribution. Probability distributions highlight that parameter values do vary across space and through time (Tucker et al., 2003) and can be used to describe both uncertainty and variability about the parameters that might occur in the unit-operation being modelled (Vose, 1998; Davey, 2011).

Although no specific information on the most suitable probability distribution for  $Fr \ 13$  risk assessment, a **RiskNormal** distribution is defined for the input parameters for the  $Fr \ 13$  unit-operations model for UV irradiation for potable water with presence of suspended solids. This distribution is very useful especially for Monte Carlo sampling of microbial risk. This is because *Normal* distribution can extend over a great range of negative infinity to positive infinity. **RiskTruncate** can be used to overcome the nonsensical values in the simulation, by setting a specified minimum and maximum value. However, other types of distribution might be more suitable if a truncated normal distribution is used (Vose, 2008).

Generally, there are about 40 theoretical probability distributions that could be also used such as Triangle and Beta-subjective (Zou, 2015). Furthermore, Davey and coworkers reported that the number of Fr 13 failures is not sensitive to a range of distributions – but, this might not always be the case (Law, 2011). One practical possibility is that these distributions can also be based on expert experience (or even opinion) (Davey, 2010; Law, 2011; Zou, 2015).

An important step in Fr 13 risk assessment is to define a failure factor (p) in terms of design reduction, and actual reduction, in viable *E. coli* contaminants in the raw and treated water.

#### 2.2.2. Fr 13 and other risk approaches

Recently the impact that fluctuations can have in physical parameters in an expected steady-value was applied to a risk assessment method by Aven and Renn (2010) and Haimes (2009, 2008) and others including Milazzo and Aven (2012). In Milazzo and Aven's study, a quantitative risk approach was used to identify the unexpected failure of the rupture of pipes in the chemical industry. The study suggested that a probabilistic approach is useful to identify risks however; uncertainties still remain as to whether data used is applicable to a specific scenario (circumstance). These authors proposed a number of techniques to overcome these drawbacks. These include using chance (uncertainty) distributions (e.g. Beta-distribution; Triangular distribution or Uniform distribution) for plant parameters and an event tree model to propagate the uncertainties for risk *p*.

This study is similar to the work of The Adelaide University researchers. However, an advantage of the Fr 13 risk framework is that it based on well-established unit-
operations modelling in chemical engineering (Foust et al., 1980; Ozilgen, 1998; McCabe et al., 2001).

The difference was they use a quantitative risk approach, together with a qualitative risk technique e.g. 'score system' (of Low, Medium, and High) to investigate the process uncertainties. Milazzo and Aven (2012) however admitted that this approach restricts attention to the most credible scenarios as this approach remains largely qualitative (subjective) relying on a 'scored' system and is therefore not rigorously quantitative (Zou, 2015).

*Fr 13* is quantitative and apparently generalizable (Davey et al., 2015) and provides all, practically possible process scenarios including failed processes. This is not available from the work of Aven and others, or, from traditional risk and hazard analyses such as *Microbiological risk assessment, HACCP*, and *HAZOP* or *Reliability Engineering*. Importantly, this is because the random element is not explicit in these risk and hazard methods.

The introduction of this new approach to risk assessment is not being expected to replace current methods, but to improve them by providing a useful, additional tool for risk assessment. Undertaking some worked examples of current *Fr 13* approach by Davey and co-workers (Cerf and Davey, 2001; Davey and Cerf, 2003; Patil et al., 2005; Davey, 2010; Chandrakash et al., 2014; Hathurusingha and Davey, 2016; Zou and Davey, 2016; Abdul-Halim and Davey, 2016; 2015), preferably in parallel with current methods, would improve understanding of the operations and outcomes of the proposed novel methods.

## 2.2.3. Fr 13 as terminology

*Fr 13* since development has been carefully defined by Davey and co-workers as a particular plant outcome behavior i.e. a probability distribution of the numerical difference between the value of a key parameter outcome and the actual instantaneous value, plus an acceptable tolerance as a design margin of safety (mathematically this is p > 0).

It is acknowledged however that Fr 13 might be generally thought of as referring to a catastrophic event (Zou, 2015). Zou and Davey (2016) suggested alternate terminologies which included those based on Root Cause Analysis (RCA) (e.g. DNV's Taproot® methodology). However, because RCA is typically undertaken after an event has occurred. Additionally, they suggested Iterative Random-impacts Assessment (IRA) to predict (and fix) probable events before they occur.

It is important to note however that the probabilistic element in *Fr 13* is to quantitatively imitate the naturally occurring chance fluctuations in unit-operations. Abdul-Halim and Davey (2016) demonstrated that chance impact through unanticipated accumulation and combination of these fluctuations could lead to failure to remove viable *E. coli* from UV irradiation for potable water production - faulty fittings or human error did not need to be invoked as an explanation.

## 2.2.4. Chance and uncertainty

Generally in probabilistic risk assessments, the probability distributions are used to reflect that parameters vary across space and through time (Tucker et al., 2003). Variations of parameters are attributed to (stochastic) chance (i.e. variation that cannot be explained). Statistical methods offer a means of doing this.

Uncertainties in system behaviour are intensified in highly networked, globally connected environments. The set of possible outcomes associated with a continuous random variable is uncountable (Miller, 2006). It also describes how the risk of extreme latencies in delivering time-critical data, applications, or services can have catastrophic consequences and explains how to avoid these events.

This uncertainty can be reduced for e.g. by increasing the number of simulation runs in the *Fr 13* simulation. Optimized sampling strategies succeed in reducing this variance efficiently at reduced computational cost (Pinto and Garvey, 2012). The desired result of *Fr 13* simulation is the statistical distribution of the possible outcome behaviours.

Normal distribution is used for symmetric continuous data, in the form of the unit normal distribution-as the distribution of a test statistic. (Unit normal distribution has zero mean and unit variance).Simple techniques for Fr 13 with refined-Monte Carlo (r-MC) modelling of microbial risks using spread sheets helps analyst to realistically reflect the uncertain nature of the scenarios being modelled.

## 2.2.5. Application of Fr 13 risk assessment

The marked increase in food-borne diseases together with an awareness of the limitations of the current assessment methods had led to the multiple needs for the development of Fr 13 risk assessment. The idea had been studied on several unit-operations, not only in food processes, as summarized chronologically in Table 2.1.

Reference		Unit-operation	Fr 13 model
1	Davey and Cerf (2003)	UHT milk sterilization	The UHT parameters ( $D_r$ , $z$ , $T$ , $t$ , $C_0$ ) was defined for the probability distribution. Failure is defined as non-sterility of a 1L pack of UHT milk. Failed scenarios of 16/100,000 were identified. Risk was shown to be 16 times greater than industrially accepted criteria (= 10 <sup>-5</sup> )
2	Patil et al. (2005); Patil (2006)	Monod fermentation	Unexpected failure was defined by washout of <i>E.</i> <i>coli</i> . Result revealed combined effect of small variations (5-15 %) of growth characteristics ( $\mu_{max}$ , $Y_{x/s}$ and $K_s$ ) highly impacted fermenter operability
3	Davey et al. (2011)	2-stage Clean-In-Place (CIP) processing	<i>Fr 13</i> was illustrated by a 2- stage CIP model. Failure defined as failure to remove proteinacious deposits on wet surfaces in an auto-set cleaning time $(t_T' < t_T)$ . Results showed for a 2-stage (T = 60 °C), 10 of 1,000 operations could fail unexpectedly. This illustrated that CIP is a combination of successful and failed operation
4	Zou and Davey (2014)	Membrane process	Membranes failure is defined as a permeate flow rate (J') less than a critical ( $J_{critical}$ ) flux. Membrane parameters ( $\Delta P$ ) and (t) were simulated with r-MC. Results revealed 4.2 % failed to achieve $J_{critical}$ at typical commercial $\Delta P$ = 344.74 kPa and t = 120 s
5	Abdul-Halim and Davey (2015; 2016)	UV irradiation for potable water	<i>Fr 13</i> risk assessment for UV irradiation for potable water for turbulent flow was illustrated. Failure is defined as the unwanted survival of viable <i>E. coli</i> . The parameters ( $I_0$ , $k$ , $Q$ ) without suspended solids presence, was simulated and revealed 16 % failed UV operations with 10% tolerance. With suspended solids present ( $I_0$ , $k$ , [ <i>conc</i> ]) results revealed 32.1 % and 43.7 % failure. UV failure is significantly affected by fluctuation in feed water flow
6	Davey (2015)	Coal-fired boiler (CFB)	<i>Fr 13</i> were used to study the fuel-to-steam efficiency of CFB. Sampling was done on 20 key input parameters, including coal feed and quality. CFB efficiency below $\eta = 77.82$ % is considered failed. Results revealed 73 failures of 10,000 iterations. Repeat simulations highlighted premixing of coal as a practical strategy to reduce vulnerability to CFB efficiency failures
7	Chandrakash et al.	3-stage CIP	The 3-stage CIP model was developed to

 Table 2.1: Summary and chronological listing of Fr 13 risk assessments.

	(2015)	processing	demonstrate <i>Fr</i> 13 risk. Failure is defined as failure to remove whey protein on metal surfaces within auto-set cleaning time $(t_T' < t_T)$ . Results showed 2 % of failure for $T = 75$ °C, despite a margin of safety
8	Davey et al. (2016)	Pitting of metals at sea	<i>Fr 13</i> was applied to assess pitting risk of metal (AISI 316L) demonstrated in the Bass Strait. Simulation was done on pitting potential ( $E_{PTT}$ ) with <i>T</i> and [ <i>Cl</i> <sup>-</sup> ]. Resuts revealed in 5,000 iterations, 463 failed as pitting initiation ( $E_{PTT} < E_{OCP}$ + tolerance%) were identified. The novel 'isorisques' is the countours of risk probability, established new atlas of pitting
9	Hathurusingha and Davey (2016)	Chemical taste taint in barramundi	Failure is defined as the chemical taint above desired threshold concentration (0.814 and 0.77, $\mu$ g kg <sup>-1</sup> ) for GSM and MIB respectively. Simulation was done for <i>Cw</i> , <i>T</i> and <i>t</i> for practical Recirculating Aquaculture System (RAS) farmed barramundi for 260 days growth. Results showed 10.10 % of all harvests identified to have taste taint as GSM, and 10.56 % as MIB, above the threshold concentration. Failure is illustrated to impact highly by harvest time.
10	Zou and Davey (2016)	Ultrafiltration and osmotic distillation (UF-OD)	Investigates vulnerability to fouling in an apparent steady-state global process of integrated cross-flow UF-OD for concentration of fruit juice. Sampling was done with plant parameters ( $\Delta P_{UF 1-1}$ and $t_{UF 1-1}$ ). Membranes fouling is defined as a permeate flux less than the operational design flux. Risk failure of the integrated two-step UF-OD is defined as an unwanted OD flux ( $J_{OD 1-2} < J_{OD 1-2}$ , required plus 3 % tolerance). Result showed a surprise fouling in 10.5 % of all operations

The University of Adelaide researchers (Cerf and Davey, 2001; Davey and Cerf, 2003; Patil et al., 2005; Davey, 2010; Chandrakash et al., 2014; Hathurusingha and Davey, 2016; Zou and Davey, 2016; Abdul-Halim and Davey, 2016; 2015) have demonstrated, as far as is known, single-handedly that standard engineering unit-operations in chemical and bio-chemical bio-processes are amenable to *Fr 13* modelling.

At present, some aspects of  $Fr \ 13$  modelling technology are currently under development. It is the present case that some research engineers cannot accept that

variability (*chance*) will play a part, or even a significant part, in the failure of unitoperations, and that its effect cannot be minimised through yet more measurements i.e. "facts" about the process (Vose, 2008). Aspects of the technology are therefore controversial in some areas.

This research focuses on predicting the failures occurring in UV irradiation for potable water using *Fr 13* modelling. The UV irradiation model is designed to follow an annular reactor with turbulent flow. The model input parameters are linked with each other as well as with the output parameter of a UV unit-operation. These equations are then incorporated into Microsoft Excel<sup>TM</sup> spreadsheet to develop SVA model of an annular reactor with turbulent flow. Input data for SVA model is obtained from published literature. A *Fr 13* risk model with r-MC is then developed which accounts for the effect of uncertainty and variability in microbiological input parameters. Simulations for the *Fr 13* risk model are performed using a Microsoft Excel<sup>TM</sup> spreadsheet with add-in @*Risk*<sup>TM</sup> with 100,000 iterations using Monte Carlo sampling of model parameters. @*Risk*<sup>TM</sup>

The quantitatively assessed risk model is used to evaluate the failures of UV irradiation for potable water. Therefore, by placing all of the information together, we can delineate gaps in the knowledge and provide estimates of the benefits of proposed research.

This new approach has advantages over *HAZOP*, *HACCP*, *Microbiological risk assessments* or *Reliability Engineering* because it is quantitative and based on principled mass and energy balances together with microbial kinetics that involve a 'whole-of-process' understanding (Davey, 2010). *Fr 13* is beneficial as all practical scenarios that could possibly exist operationally can be quantified, including all chance of failures (Davey, 2010; 2011; Davey and Cerf, 2003).

Moreover published research has underscored that currently used engineering risk approaches (i.e. single-value-best assessments plus sensitivity analyses) actually downplay the real risks of bio-process failure and micro-organism survival. That is, the true risk of plant failure is actually significantly greater than can be currently assessed (Cerf and Davey, 2001; Davey and Cerf, 2003). This is undesirable and has motivated this new field of risk research.

*Fr 13* failure modelling uses a refined-Monte Carlo random sampling of each probability distribution of process parameters in the unit-operation to produce a number of practical operating scenarios. Each probability distribution is sampled in a manner that reproduces the distribution's shape. The advantages of using a refined-Monte Carlo for *Fr 13* risk analysis over other simulation techniques include (Vose, 2008; Davey, 2010):

- i. The distribution of the model's parameters do not have to be approximated in any way
- ii. Correlation and other interdependencies can be taken into account
- iii. The level of mathematics required is basic (although complex)
- iv. Software is commercially available to automate the tasks

- v. Complex mathematics can be included (e.g. power functions, logs, IF statements, etc)
- vi. Because *Fr 13* risk assessment uses a widely recognized refined-Monte CarloAssessment is as a valid technique, so its results are more likely to be acceptedvii. The behaviour of the model can be investigated with great ease
- viii. Changes to the model can be made very quickly and the results compared with previous models.

The distribution of the values calculated for each outcome therefore reflects the probability of the values that could occur practically. The *Fr* 13 simulator uses a random number generator (Davey, 2011; Vose, 2008).

Unlike other research which uses single-value-best assessments plus sensitivity analyses as an input to the process to obtain the output (Patil, 2006; Davey, 2011), this new research project will use refined-Monte Carlo simulation to actual unit-operations of UV irradiation for potable water production. This method is advantageous over the single value method because the results obtained will be both 'quantitative' and 'process-based'. This method offers a powerful way of assimilating both *uncertainty* (i.e. the process facts) and *variability* (effect of chance on process parameters) into a realistic appreciation of total risk in a problem (Vose, 2008; Davey and Cerf, 2003).

Further, the probabilistic elements in Fr 13 provide a quantitative picture of all mathematically practical possibilities of process scenarios, including failures. The quantitative capacity of this framework to give outcomes to distinguish the effect of targeted intervention strategies or design changes in second-tier simulations on plant behavior is a major advantage. Vulnerability to failure can be reduced through second-tier simulations to make physical changes or suggest intervention strategies to a process or operating practices (Chandrakash et al., 2015; Zou and Davey, 2016). This can be applied at both analysis and synthesis stages.

An important drawback of the Fr 13 framework to date however is that it is has been largely limited to one-step (single) unit-operations. Therefore, the benefit in applying this approach or developing the framework to a multi-step chemical unit-operations and processes is not known yet to be considered a useful tool.

## 2.2.7. Fr 13 risk assessment for UV irradiation unit-operation

In *Fr 13* modelling, what primarily is required is a practical and unambiguous definition of failure of process or product in unit-operations (Davey, 2010).

In UV irradiation for potable water production, this is an unacceptable (unsafe or undesirable) level of the survival of unwanted pathogenic or spoilage viable contaminant micro-organisms in the water produced.

This research focuses on predicting the vulnerability to failure of UV irradiation for potable water using *Fr 13* modelling. Whilst it is acknowledged probabilistic approaches have been applied by others to the inactivation of contaminant micro-organisms, for example to simulating simple heating effects on bacterial death (Ferrer et al., 2006) and although a number of researchers around the world are working on risk assessments (e.g. Ferrer et al. (2006); Min and Choi (2009); Gudmundsson and Kristbergsson (2009)) none as far as we are aware, have taken the crucial step of linking the microbial aspects with aspects of process using quantitative risk assessments in chemical and bio-chemical engineering unit-operations.

## 2.3. Ultraviolet irradiation

## 2.3.1. UV light

Sunlight has been reported by Downes and Blunt (1877) to have the effect on inactivating bacteria (Hockberger, 2002; Masschelein and Rice, 2002). However, the effect of inactivating bacteria was not achieved by sunlight, which only play a small part but of UV rays. UV ray is the region of the electromagnetic spectrum that lies between X-rays and visible light as shown in Fig. 2.2.

The electromagnet spectrum is divided into four regions; Vacuum UV, UV-C, UV-B and UV-A which ranges from 100 nm to 400 nm.

Ultraviolet germicidal irradiation (UVGI) is a term originally adopted from the International Commision on Ilumination (CIE) for spectral bands. The CIE has designated UVGI spectrum which ranges from 200 nm to 400 nm; UV-C (200 nm-280 nm), UV-B (280 nm-315 nm) and UV-A (315 nm-400 nm) (Kowalski, 2009; Sliney and Chaney, 2001; Anon., 2006; Das, 2002).



Fig. 2.2: UV spectrum (Adapted from Anon., 2006)

A summary of the spectrum ranges is given in Table 2.2. Primarily, inactivation of micro-organisms occurs in the UV-B and UV-C region. Unlike UV-B and UV-C light, UV-A light requires long exposure times to be effective (Anon., 2006). Moreover, UV radiation below 320 nm can cause photochemical reactions or actinic. Actinic wavelengths involve energies that are able to provoke direct chemical changes in the irradiated molecules (activation, ionization, dissociation, etc.), and to promote biological changes in the systems accordingly (Masschelein and Rice, 2002). However, the practice of water disinfection with UV light is more known as it is mainly concerned with the UV-C range, defined at 254 nm.

Туре	Range	Comment
UV-A	400 to 315 nm	Between 400 and 300 nm, sometimes called near UV
UV-B	315 to 280 nm	Sometimes called medium UV
UV-C	280 to 200 nm	Range to be considered in more detail in water. At 254nm can
		lethally be damaging to micro-organisms

**Table 2.2:** Summary of UV spectrum range.

## 2.3.2. Mechanism of UV irradiation

The mechanism in which UV irradiation inactivates the viable micro-organism is by irreparable damage to the cellular DNA. At 254 nm, UVGI causes dimerization of adjacent thymine monomers on the same strand of DNA. This prevents normal DNA transcription and replication to occur. Formation of many thymine dimmers along a single DNA strand makes replication very difficult (USEPA, 1986; Brock and Madigan, 1991) thus, resulting in inactivation of micro-organisms (Block, 1983; Nguyen, 1999; Cano and Colome, 1986). The wavelength of 254 nm is the optimum absorbance by nucleic acids (Qasim, 1999; USEPA, 1986) and is primarily the wavelength used by most UV irradiation technology (Harm, 1980; USEPA, 1986; Amos, 2007; Nguyen, 1999).

However, there is a possibility of cell photoreactivation with UV irradiation treatment (Nebot Sanz et al., 2007; Zimmer and Slawson, 2002). Photoreactivation is the phenomenon whereby inactivated micro-organisms regain activity through repair of pyrimidines dimers in the DNA under near UV and visible light exposure ranging from 310 to 480 nm (Nebot Sanz et al., 2007). The repair of bacteria after exposure to UV light is not universal. Some organisms seem not to have the capability of repair (i.e. *Haemophilus influenzae, Diplococcus pneumoniae, Bacillus subtilis, Micrococcus radiodurans*, viruses); others have shown the capability of photorepair (i.e. *Streptomyces* spp., *Escherichia coli* and related enterobacteria, *Saccharomyces* spp., *Aerobacter* spp., *Erwinia* spp., *Proteus* spp.) (USEPA, 1986). However, viruses, when damaged by UV irradiation, have no repair mechanisms (Masschelein and Rice, 2002).

To avoid photorepair, an additional UV dose was required (Masschelein and Rice, 2002). The amount of cell damage and subsequent repair is directly related to the UV dose and the amount of repair will depend on the dose (intensity) of photoreactivating light (Das, 2002). In an experiment on repair mechanisms of coliform bacteria done by (Lindenauer and Darby, 1994) after exposure to higher doses, coliform bacteria exhibit less or no repair at all. This is because the higher dose causes greater number of damaged sites. Also, (Groocock, 1984) discovered to prevent from photorepair to occur, exposure to light (300 to 500 nm) must occur a short time after exposure to germicidal light (within 2 to 3 hours). More complete photorepair may last up to one week for *E. coli* (Masschelein and Rice, 2002).

## 2.3.3. UV irradiation for potable water production

Potable water can be produced by UV inactivation of pathogens. Inactivation is an effective barrier to many pathogens (especially bacteria) during water treatment process. Despite the fact that it can selectively inactivate contaminants, poorly treated water can cause waterborne diseases.

Three categories of human enteric contaminants or contaminants that are transmitted by the faecal-oral route were discovered as the most harmful to humans that can cause waterborne diseases. These contaminants consist of: bacteria, viruses and anaerobic cysts (Parsons and Jefferson, 2009; Das, 2002). Diseases that can be caused by these contaminants include typhoid, cholera, paratyphoid, poliomyelitis and infectious hepatitis (Das, 2002). In fact, if not controlled, these diseases can reach epidemic proportions (Pilkington, 1995).

Chlorine is the most widely used disinfection method because of its long history in literature and the effectiveness in inactivation of micro-organisms in drinking water (Pilkington, 1995; White, 1999). However, many concerns have been put on the byproducts, which some was shown to have potential health concern (i.e. carcinogenic) to human (Fiessinger et al., 1985; Dunnick and Melnick, 1993; Clark and Sivaganesan, 1998; Hua and Reckhow, 2007). For this reason, many developments have been done for alternative inactivation technologies and with an increase interest in a much economical water inactivation unit (i.e. UV irradiation, membrane filtration, electrochemical, etc). Physical inactivation by using heat is commonly used in the beverages and dairy industry by heating the water to its boiling point. However, heating is not of practical use for treating large volumes of water because it is not economical (Das, 2002).

UV irradiation for potable water has become the most promising advancing technology in water industries supported by decades of fundamental and applied research and practice since its earliest scientific observations of the germicidal effects of radiation by sunlight on micro-organisms by (Downes and Blunt, 1877; Hockberger, 2002; Masschelein and Rice, 2002). However, only less than 10 % of the total sunlight intensity that reaches the surface of the earth is UV light, with little active radiation for inactivation of micro-organisms in water available (Masschelein and Rice, 2002). Therefore high intensity UV irradiation technologies were developed for water inactivation purpose.

The first large-scale application of UV light, at 200 m<sup>3</sup> day<sup>-1</sup>, for drinking water disinfection was in Marseille, France from 1906 to 1909 (Masschelein and Rice, 2002; Hijnen et al., 2006). However, comparative benefits of UV irradiation and chemical disinfection occurred resulting in confined development for UV irradiation for potable

water production. Early UV irradiation process have problems with the operations i.e. costs, maintenance of the equipment, and aging of the lamps (Masschelein and Rice, 2002; Hijnen et al., 2006).

Due to lower cost and simpler operations, micro-organisms inactivation using chlorine was preferred (Hoyer, 2004). UV irradiation have become the methods of choice again. The re-emergence of UV irradiation by the water industry is also because of the regulatory impacts to other inactivation methods and very quickly gained popularity in the water industry as a method for micro-organisms inactivation over the next several years.

## 2.3.4. Advantages and disadvantages of UV irradiation for potable water

UV irradiation has now emerged as a widely used method as an alternative method for chlorination for inactivation of micro-organisms in potable water production (Hijnen et al., 2006; Severin et al., 1983; Cassano et al., 1995; Bolton, 2000; Elyasi, 2009; Ye et al., 2007; Koutchma et al., 2009; Masschelein and Rice, 2002; Das, 2001; 2002). Advantages and disadvantages of UV irradiation are summarised in Table 2.3: Table 2.3: Advantages and disadvantages of UV irradiation for potable water production

as an alternative to chlorination method.

Advantages		Disadvantages		
1.	Cost are competitive to chlorination (Pilkington, 1995; Kim et al., 2002; Okpara et al., 2011)	1.	At lower UV dose, some micro-organisms might not be effectively inactivated (Johnson et al., 2010; Nguyen, 1999)	
2.	No on-site storage of chemicals are required, eliminating the risk for the operators and the safety measures and equipment for handling chemicals are not needed (Masschelein and Rice, 2002; USEPA, 1999)	2.	Targeted micro-organisms can sometimes repair and reverse destructive effects of UV irradiation through photo-reactivation and dark repair (in absence of light) (Nguyen, 1999; Amos 2007)	
3.	It is non-intrusive, produces no noticeable adverse odour or taste (Kiely, 1998)	3.	Turbidity and total suspended solids (TSS) in water can also reduce the effectiveness of UV irradiation (USEPA, 1999)	
4.	Effective at inactivating most bacterial and viral contaminants (USEPA, 1999)	4.	A preventive maintenance program is also necessary to control fouling tube (USEPA, 1999)	
5.	Has a low energy and minimal space requirement (Nguyen, 1999; USEPA, 1999; Amos, 2007)			
6.	Since it is a physical process, any possible adverse effect will stop when the process stops (Amos, 2007)			
7.	There are no harmful by products whereas the conventional chemical disinfection methods have been questioned to have toxic by-products that are harmful to living creatures (van Mourik et al., 2010; Das, 2002; Ward and DeGrave, 1978; Hua and Reckhow, 2007)			

#### 2.3.5. UV reactors configuration

Majority of current UV irradiation units in water treatment are open channel, modular design which can be divided into two (2) groups as shown in Fig. 2.3, (a) vertical lamp configuration and (b) horizontal lamp configuration. For the vertical configuration, the principal flow direction is perpendicular to staggered lamp while the principal flow is parallel to the lamp axes in the horizontal configuration. These configurations are suitable for water treatment for large quantities of liquids and low absorption coefficients (i.e. wastewater) (Ye, 2007; Chiu et al., 1999; Lyn et al., 1999). Another type of UV reactor is a thin film annular reactor as shown in schematic in Fig. 2.4. This UV reactor produces an annular thin film between two concentric cylinders and is more suitable for inactivating pathogens in water with high absorption coefficients (i.e. juices) (Ye, 2007).

An annular reactor was chosen in this study to illustrate Fr 13 risk assessment for turbulent flow pattern in Chapter 4 onwards.. Turbulent flow occurred when the two concentric cylinders are fixed, flow pattern can be Poiseulle flow or turbulent flow depending on the flow rates (Ye, 2007).



**Fig. 2.3:** Schematic diagram of an open-channel UV irradiation with (**a**) vertical lamp configuration (**b**) horizontal lamp configuration (Adapted from Ye, 2007)



**Fig. 2.4:** Schematic diagram of a thin film annular-reactor between two concentric cylinders (Adapted from Ye, 2007).

## 2.4. Shortcomings

The previous research studies do not allow for the following:

- 1. Use a single value of input instead of a distribution of values to obtain the output
- 2. Do not account for the uncertainty and variability in the input parameters.

This research will therefore be the first attempts to quantify the effects of uncertainty and variability in the model input parameters of UV irradiation for potable water.

## 2.5. Summary and conclusions

From the review of the literature, the following important factors emerge which are relevant to this study:

- 1. The terminology of 'risk' and 'risk assessment' are still evolving because there are still not one universally satisfactory definition for 'risk assessment'
- 2. The *Fr 13* risk framework has been successfully developed and applied to steady-state, single-step foods and engineering unit-operations to gain new insight into how naturally occurring, random fluctuations within process parameters can lead to unexpected (surprise) failures in a well-operated, well-maintained plant
- 3. A major advantage claimed for *Fr 13* is that, because it provides quantitative insight into underlying unit-operations behaviour and plant outcomes, it can be used to proposed process intervention strategies and re-design of physical plant i.e. second-tier studies to reduce risk, and it can be applied at both analysis and synthesis stages. An important drawback of the *Fr 13* framework to date however is that it is has been applied to one-step (single) unit-operations
- 4. Fr 13 framework is a powerful new tool to successfully manage the impact of uncertainty and variability in any real system. The application of this novel methodology could help to close gaps in knowledge and provide more accurate parameter estimations, and therefore prove to be helpful in allocation of the available resources for in-depth research of the microbiological input parameters

36

- 5. UV irradiation is a widely accepted alternative to chlorination for potable water production to inactivate pathogens in water. Presence of *E. coli* in treated water indicates failed UV processes
- 6. *Fr* 13 risk assessment is illustrated using a developed turbulent flow model in an annular reactor
- Despite the apparent need of failure vulnerability to achieve greater insight into practical operations of UV irradiation, none has been reported
- 8. The *Fr 13* framework appears relevant for a novel risk analysis of one- and two-step UV irradiation for potable water.

In the next chapter, a preliminary one-step UV irradiation model for laminar flow is synthesized using SVA and then evaluated for its performance using Fr 13 with a r-MC simulation. Simulation results for targeted intervention strategies are discussed.

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# **CHAPTER THREE**

# FRIDAY 13<sup>TH</sup> FAILURE MODELLING: A NEW QUANTITATIVE RISK ASSESSMENT OF UV IRRADIATION FOR POTABLE WATER

# FRIDAY 13<sup>TH</sup> FAILURE MODELLING: A NEW QUANTITATIVE RISK ASSESSMENT OF UV IRRADIATION FOR POTABLE WATER

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By signing the Statement of Authorship, each author certifies that:

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#### Abstract

UV irradiation is an alternative to widely used chemical disinfection to produce potable water. Failure of a well-run, well-maintained UV plant can lead to catastrophic and enduring public health effects, with or without fatalities. Failure is defined as the unexpected survival of levels of pathogenic *Escherichia coli*. *Friday* 13<sup>th</sup> failure modelling (Fr 13) is an emerging method for new quantitative risk assessments of unexpected failure in process plant due to 'within system' chance (stochastic) changes. In this original research a new Fr 13 risk assessment of a simplified unit-operations model for UV irradiation for potable water is presented for the first time. A comparison is made between the predictions from a traditional, single point assessment and Fr 13 model using established UV inactivation kinetics for E. coli. A process risk factor (p) is synthesised in the Fr 13 model and is solved using a refined Monte Carlo simulation with Latin Hypercube sampling. Results reveal that 47 in every 10,000 continuous UV operations can fail unexpectedly with a tolerance of 10% on the design level of reduction in E. coli. This translates, on average, to an unexpected survival of E. coli each 0.58 years of continuous operation. This new insight is not available from traditional assessments, with or without sensitivity analyses. Practical methods of reducing unexpected failure and improving process technology in UV plant for potable water are briefly discussed.

#### 3.1. Introduction

UV irradiation provides an alternative to widely used chemical disinfection to economically produce large volumes of potable water (Kim et al., 2002). It is effective in the inactivation of both bacterial and viral contaminants. Other advantages include that it is non-intrusive, produces no noticeable adverse odour or taste (Kiely, 1998; Nguyen, 1999), has low energy and space requirements compared with chemical disinfection (Amos, 2007; Amos et al., 2001), and is generally more cost effective (Kim et al., 2002; Okpara et al., 2011). The cost of UV irradiation has decreased over recent years due to improvements in lamps and plant designs (Okpara et al., 2011).

Because failure of UV plant can lead to enduring public health effects, with or without fatalities, a quantitative understanding of process risk is important. Current risk assessment methods (Haas, 1983; Medema et al., 2003; Okpara et al., 2011; Regli et al., 1991; Teunis et al., 1997) however lack a sense of 'process' and are semi-quantitative (Davey, 2010). Often a 'risk' is reported when what is actually meant is a 'hazard' (Davey, 2010).

Of emerging research interest is the notion that no matter how good the design and operation of process plant there will be an occasional, unexpected failure. This practically observable and widely acknowledged phenomenon in otherwise well-operated, well-maintained process plant has been titled *Friday 13<sup>th</sup> failure (Fr 13)* by Davey and co-workers (Cerf and Davey, 2001; Davey, 2011a; 2011b; Davey et al., 2011). *Fr 13* is the result of an accumulation of small variations in key process parameters that combine in one direction to leverage unexpected changes in process conditions. Often 'human error' or 'faulty fittings' are falsely blamed (Cerf and Davey, 2001; Davey, 2001; Davey, 2011; Davey, 2001; Davey, 2010; 2011b; Langer, 2008).

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The principal aim of this original research is to report for the first time a quantitative risk assessment of unexpected failure of UV irradiation for potable water using the new Fr 13 failure modelling. An advantage highlighted over traditional methods of Fr 13 is an enhanced understanding of risk in UV irradiation for potable water which can be used to safeguard plant and public health, and guide improved process technologies.

#### **3.2.** A model for UV irradiation

An essential first step is the synthesis of an adequate unit-operations model for UV irradiation. This requires a marriage and integration of equations for UV lamp intensity, residence time of the water to the lamp, and; kinetics of inactivation of water-borne contaminants. The criteria for an adequate model must include (Amos et al., 2001):

- Accuracy of prediction against observed data
- Ease of synthesis and use i.e. relative complexity of *economy/elegance*
- A generalized form applicable to a wide range of micro-organisms.

UV dose is the key parameter. This can be calculated from exposure time of the water (*t*) to lamp intensity (*I*) (Amos, 2007; Amos et al., 2001; Loge et al., 1996) such that:

$$[dose] = It \tag{3.1}$$

where all symbols used are defined in the Notation at the end of this paper.

The kinetics of UV inactivation are widely assumed to be a first-order reaction with respect to dose (Amos, 2007; Amos et al., 2001; Hijnen et al., 2006; Loge et al., 1996). Mathematically this can be represented as:

$$\ln(\frac{N}{N_0}) = -kIt = -k[dose]$$
(3.2)

or conveniently to base  $log_{10}$ :

$$\log_{10}(\frac{N}{N_0}) = \ln(\frac{N}{N_0})/2.303$$
(3.3)

From Equation (3.2) a plot of  $\ln (N/N_0)$  versus UV dose gives a straight-line through the origin with slope, *k*.

A widely used indicator pathogen in potable water production is *Escherichia coli* (Amos, 2007; Amos et al., 2001).

Importantly, any suspended solids in the water will act as a shielding-agent to dose and will result in low UV efficacy (Amos et al., 2001; Loge et al., 1996; Nguyen, 1999). Amos *et al.* (2001) demonstrated the Davey-Linear Arrhenius equation to be the most adequate for description of UV irradiation of viable *E. coli* in comparison with the classical log-linear, Square-Root and  $n^{\text{th}}$  Order Polynomial models. This finding was based on extensive analyses of residual plots of experimental data and appropriate criteria including: parsimony and ease of use and ready integration with additional equations to describe a UV irradiation unit-operation.

The Davey-Linear Arrhenius for UV inactivation of *E. coli* in the presence of suspended solid is given by:

$$\ln k = C_0 + C_1[dose] + C_2[dose]^2 + C_3[conc]$$
(3.4)

This equation is said to be 'additive' in form i.e. [*dose*] and [*conc*] appear to act independently to effect inactivation (Amos, 2007; Daughtry et al., 1997). It is widely

applied to general inactivation of micro-organisms (McMeekin et al., 1993; Bruin and Jongen, 2003; Min and Choi, 2009).

Equation (3.1) through (3.4) establishes the simplified unit-operations model for UV irradiation of *E. coli* for potable water.

### **3.3.** *Friday* 13<sup>th</sup> failure model

#### 3.3.1. Defining UV Failure

An essential element of a *Fr 13* quantitative risk assessment is a clear definition of a process (or product) risk factor, p (Davey, 2010; 2011b). A suitable risk factor for UV irradiation can be defined as the design  $\log_{10}$  reduction in viable *E. coli* together with an acceptable level of *%-tolerance* such that:

$$p = -\% \ tolerance + 100[1 - \frac{\log_{10}(\frac{N}{N_0})}{\log_{10}(\frac{N}{N_0})}]$$
(3.5)

where  $\log_{10}(\frac{N}{N_0})$  is an instantaneous value of  $\log_{10}(\frac{N}{N_0})$ . This is computationally convenient because as can readily be seen from Equation (3.5) for all p > 0 UV fails.

### 3.3.2. Simulating Friday 13<sup>th</sup>

In simulation of a Fr 13 model key parameters are defined by a distribution of values, the mean of which generally agrees with the traditional single point, or single value

assessment (SVA) (Cerf and Davey, 2001; Davey, 2011b; Patil, 2006; Patil et al., 2005). The parameter distribution is carefully defined so as to cover all practical values that might occur in day-to-day operations (Cerf and Davey, 2001; Davey, 2010; 2011a; 2011b; Davey et al., 2011; Patil, 2006). A refined Monte Carlo sampling is used with Latin Hypercube sampling to ensure that the random samples within each probability distribution cover the entire range of the distribution (Davey, 2011b; Vose, 2008). To ensure the output distribution is Normal a minimum number of random samples are necessary; this usually means 1,000 to 50,000 samples will be needed (Davey K R - unpublished data). It is a simple matter to establish this visually with most software.

The 'within system' practical variation (sdev) in the lamp intensity is assumed at 1% and for each of the concentration of shielding agent [*conc*] and residence time, *t*, 5%.

The selected distributions for *I*, [*conc*] and *t* are defined as: **RiskNormal**(mean, sdev, **RiskTruncate**(minimum = mean - 2\*sdev), (maximum = mean + 2\*sdev))). For example, for the lamp, this means a mean intensity of 11,940 with sdev of 120 and a minimum 11,700 and maximum 12,180  $\mu$ W cm<sup>-2</sup> is used. The distributions are truncated to indicate that the chance of a practical process value being outside the range is (zero) negligible. A practical process tolerance of 10% on the required log<sub>10</sub> reduction of viable *E. coli* is assumed.

Calculations were performed in Microsoft Excel<sup>™</sup> with a commercially available add-on @*Risk*<sup>™</sup> (pronounced at-risk) version 5.7 (Palisade Corporation). This is convenient because Excel has nearly universal use, and therefore makes communication of results streamlined.

Simulations were used to identify practical process events that give rise to UV failure i.e. for all values of the risk factor p > 0.

#### 3.4. Results

Table 3.1 presents a summary comparison of the *Fr 13* and traditional single point (SVA) assessments for UV irradiation using the Davey Linear-Arrhenius kinetics for inactivation of viable *E. coli* in water with suspended solids, and a process tolerance of 10% on the design level of reduction. The UV process parameters are given in column 1 of the table. These are the lamp intensity, suspended solids concentration and residence time. Traditional SVA calculations are presented in column 2.

10,000 random samples of each input distribution (*I*, [*conc*] and *t*) were used. This means calculations will have been performed on all possible combinations of practical process scenarios that could occur in the UV unit-operation. The values in column 3 of the table are for one only scenario of these 10,000. For this scenario shown it can be seen that p > 0, indicating UV failure.

**Table 3.1:** Comparison of traditional single point (SVA) and *Fr 13* risk assessments for UV irradiation for potable water with the Davey Linear-Arrhenius equation for inactivation of *E. coli*.

<b>UV Parameter</b>	SVA <sup>*</sup>	Fr 13 <sup>&amp;</sup>	
$I(\mu W cm^{-2})$	11940	11811.66895	RiskNormal(11940, 120, RiskTruncate( 11700, 12180))
$[conc](gl^{-1})$	0.115	0.11638	RiskNormal(0.115, 0.006, RiskTruncate( 0.104, 0.127))
<i>t</i> (s)	1.90	1.71616	RiskNormal(1.9, 0.095, RiskTruncate( 1.710 2.090))
[dose] (µWscm <sup>-2</sup> )	22686.00	20270.68555	Equation (3.1)
$k (\mu W^{-1} s^{-1} cm^2)$	0.0004139	0.00041395	Equation (3.4)
$\ln N/N_0$	-9.391	-8.39101	Equation (3.2)
$\log_{10} N/N_0$	-4.078	-3.64351	Equation (3.3)
р		0.64672	Equation (3.5)

\* SVA = Traditional single point, or, Single Value Assessment

<sup>&</sup> With Latin Hypercube sampling

A total of 47 failures were identified in the 10,000 scenarios. Five of these are presented in Table 3.2 where it can be seen all have a value of p > 0. This table shows combinations of the practically realizable values of the UV process parameters that led to failure to achieve the design reduction in level of viable *E. coli* (with the assumed tolerance of 10%). In the table, row 2, shows the combination of randomly sampled values for, respectively,  $I = 11811.66895 \,\mu\text{Wcm}^{-2}$ ,  $[conc] = 0.11638 \,\text{g I}^{-1}$  and  $t = 1.71616 \,\text{s}$ , resulted in a corresponding value of p = 0.64672; this is the particular scenario given in Table 3.1.

Ι	[conc]	t	р
(µWcm <sup>-2</sup> )	( <b>g l</b> <sup>-1</sup> )	<b>(s)</b>	
11741.15137	0.11916	1.71136	1.42826
11811.66895	0.11638	1.71616	0.64672
11740.73730	0.11451	1.73133	0.39807
11863.45508	0.11532	1.71656	0.23402
11890.02539	0.10521	1.71595	0.065038

Table 3.2: 5 failures from 47 in 10,000 UV irradiation scenarios.

#### 3.5. Discussion

If each simulation scenario is thought of as an operational day, then an unexpected *Fr 13* failure in UV irradiation would occur once every (10,000/365.25/47 =) 0.58 years on average despite best operation and maintenance. These would not, of course, be spaced equally in time.

As the process *%-tolerance* is increased the model can be used to show the number of failures will reduce, and conversely, increase with a reduced *%-tolerance*.

This implies a practical method of reducing Fr 13 failure in UV irradiation is to reduce the variance in key input parameters through improved process control. An

apparent exponential dependence of failure rates suggests that increased costs for improved process control could be readily justified.

A practical question is how the value of the risk factor p will be affected through improved process control: the answer is, some experimenting will need to be done using the *Fr 13* model. In more general situations knowledge from experienced operators or 'experts' could be drawn on to devise a process-specific distribution (Davey, 2010; 2011b).

The general principle of *Fr 13* modelling has been illustrated i.e. to calculate the combined impact of chance (variability) in key parameters on the probability distribution (likelihood) of possible process outcomes. Traditional SVA approaches, with or without a sensitivity analysis, do not separate these (Hoffman and Hammonds, 1994; Ria and Krewski, 1998) and therefore cannot give practical insight into unexpected UV failures. SVA estimates of risk may actually give a greater sense of process safety than is the case (Cerf and Davey, 2001; Davey, 2011b); this is tacitly acknowledged as many processes involve deliberate over-treatment which is wasteful not only in energy, but plant costs.

The valuable insight gained with  $Fr \ 13$  risk modelling into UV irradiation for potable water over traditional methods has been to quantitatively identify fail scenarios that are probable. Importantly,  $Fr \ 13$  can be used as a second-tier simulation to investigate any proposed physical changes to the process (Davey, 2011b).

#### 3.6. Conclusions

A new *Fr 13* quantitative risk model has revealed that failure of UV irradiation for potable water, defined by unwanted viable *E. coli* post-treatment, can result from chance

(stochastic) variability in key process parameters. The number of failures is related to the combined effects of variance about process parameter mean values.

Reducing the variance in key parameters, through for example improved process control, whilst potentially costly, can minimize likelihood of UV failures.

Fr 13 modelling can be used to quantitatively assess reduced risk of UV failures from proposed changes in process control or design, or intervention strategies, and therefore can be used to guide improvements in process safety and technology. This is because Fr 13 modelling is a significant elaboration on current and limited SVA analyses as it produces all possible outcomes of UV operations.

#### Notation

The number in parentheses after description is the equation in which the symbol is defined or first used.

- *C<sub>i</sub>* Davey Linear-Arrhenius coefficients for UV shielding of *E. coli* (Amos, 2007):  $C_0 = -6.334; C_1 = -7.71 \times 10^{-5}; C_2 = 7.23 \times 10^{-10}; C_3 = -0.685$  (3.4)
- k rate coefficient for UV inactivation,  $\mu W^{-1} s^{-1} cm^2 (3.2)$  and (3.4)
- N number of viable *E. coli* at t = t (3.2), (3.3) and (3.5)
- $N_0$  number of viable *E. coli* at t = zero (3.2), (3.3) and (3.5)
- [*conc*] solids (shielding) concentration, 0.115 g  $L^{-1}$  (3.4)
- [*dose*] UV dose, It,  $\mu$ W s cm<sup>-2</sup> (3.1), (3.2) and (3.4)
- *I* UV lamp intensity, 11,940  $\mu$ W cm<sup>-2</sup> (3.1) and (3.2)
- t exposure time, 1.9 s (3.1) and (3.2)
- *p* risk factor, dimensionless (3.5)

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# **CHAPTER FOUR**

# A FRIDAY 13TH RISK ASSESSMENT OF FAILURE OF ULTRAVIOLET IRRADIATION FOR POTABLE WATER IN TURBULENT FLOW

# A FRIDAY 13TH RISK ASSESSMENT OF FAILURE OF ULTRAVIOLET IRRADIATION FOR POTABLE WATER IN TURBULENT FLOW

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By signing the Statement of Authorship, each author certifies that:

- i. the candidate's stated contribution to the publication is accurate (as detailed above);
- ii. permission is granted for the candidate in include the publication in the thesis; and
- iii. the sum of all co-author contributions is equal to 100 % less the candidate's stated contribution

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#### Abstract

Ultraviolet (UV) irradiation for potable water is an important alternative to widespread disinfection methods such as chlorine. Failure of UV irradiation to reduce levels of viable contaminants can lead to enduring health effects, with or without fatalities. Here a new risk assessment of failure of UV irradiation for potable water in turbulent flow in a series annular-reactor is presented using the Friday 13<sup>th</sup> (Fr 13) methodology of Davey and coworkers (Food Control 29(1), 248-254, 2013). The aim was to demonstrate the effects of stochastic (random) changes in UV parameters on plant failure. Failure is defined as unexpected levels of survival of Escherichia coli, a species of fecal bacteria widely used as an indicator for health risk. The assessment is based on a unit-operations model of UV irradiation together with extensive experimental data of Ye (2007). A failure factor (p) is defined in terms of the design reduction and actual reduction in viable E. coli contaminants. UV irradiation is simulated using a refined (Latin Hypercube) Monte Carlo (r-MC) sampling. Illustrative results show 16 % of apparent successful operations, over the long term, can fail to achieve the design reduction in viable E. coli of  $10^{-4.35}$  due to stochastic effects. The analysis is shown to be an advance on current risk assessments because it produces all possible practical UV outcomes. Implications of Fr 13 methodology for practical re-design and targeted physical changes to UV plant for improved reliability and safety is discussed.

#### Keywords:

Ultraviolet (UV) irradiation for potable water; UV risk analysis; stochastic failure of UV irradiation; Friday 13<sup>th</sup> failure modelling of UV; Friday 13<sup>th</sup> risk modelling

### Highlights

- Stochastic effects identified as cause of failure of ultraviolet (UV) irradiation
- UV shown to be a continuous mix of successful and unsuccessful operations
- Approach can be used to quantitatively assess risk of failure and improve safety
- Immediate benefit to designers and operators of UV equipment for potable water

#### 4.1. Introduction

Ultraviolet (UV) irradiation for production of potable water is an increasingly attractive alternative to widely used chemical disinfectants, such as chlorine (Amos et al., 2001). Advantages of UV irradiation include that it: adds nothing to the water (compared to chemical disinfection); inactivates both bacterial and viral contaminants; produces no harmful by-products; does not alter the taste or properties of the water, and; is increasingly cost effective (Okpara et al., 2011; Amos et al., 2001). Because of these advantages UV irradiation is increasingly relied on globally to produce potable water, and is often required to be in continuous operation for prolonged periods. Failure of UV irradiation to reduce viable contaminants to a safe level can lead to enduring public health effects, with or without fatalities. A quantitative risk understanding of UV irradiation plant is therefore important.

In recent years Davey and co-workers (Davey et al., 2011; 2012; 2013; Davey, 2010; 2011; Patil et al., 2005) have illustrated a novel risk assessment titled *Friday 13<sup>th</sup>* (*Fr 13*). The idea is based on the practical notion that despite best design and operation of a continuous process there will be an occasional, unexpected and surprise failure that cannot be attributed to human error or faulty fittings (Cerf and Davey, 2001). A key insight is that an accumulation of stochastic (random) changes in otherwise well-operated continuous plant parameters can lead unexpectedly in one-direction and leverage significant sudden change in process or product. Published case studies include a sudden and unexpected change from sterile milk to non-sterile product (Davey and Cerf, 2003); from stable to unstable operation with fermenter 'washout' (Patil et al., 2005); from clean to unclean (CIP) processing (Davey et al., 2011; 2013); and more generally, from safe to unsafe (Davey et al., 2012).

Current food safety management tools and alternative risk assessments include *Microbiological risk assessment* (CAC, 1998), HACCP (*Hazard Analysis Critical Control Point*), HAZOP (*HAZard and OPerability*) and *Reliability Engineering* (O'Connor et al., 2002). Importantly, although these methods have been adapted widely they cannot be used to understand and reduce random effects, with either more study or measurement (Anderson and Hattis, 1999; Vose, 2008). This is because this critical parameter in these assessments is omitted, or strictly, 'hidden'. This is true also of the recent assessment of Riverol and Pilipovik (2014) who addressed process 'failure frequency' with a case study on milk pasteurization. This work is not developed from widely used unit-operations principles in foods processing (see for example Foust et al., 1980; Schwartzberg and Rao, 1990; Ozilgen, 1998) and does not appear to be generalizable; it has much in common with *Reliability Engineering*. In contrast, an advantage with *Fr 13* assessments is that both the facts about the process and the effects of random changes in parameters are separated (Hoffman and Hammonds, 1994; Ria and Krewski, 1998; Davey et al., 2012; 2013). This is more mathematically correct and permits the effect of each to be studied.

The principle of Fr 13 is that it is predicated on the underlying unit-operations model together with a practical definition of product failure and a refined Monte Carlo (r-MC) simulation (Davey, 2011). Importantly, published findings from Fr 13 assessments have generally underscored that current risk assessments actually downplay the real risks in bio-process failures and survival of unwanted micro-organisms (Cerf and Davey, 2001; Davey et al., 2011; 2012; 2013; Patil et al., 2005).

A seminal *Fr 13* assessment of UV irradiation was presented by Davey and coworkers (2012) for *Escherichia coli* in the presence of suspended solids (as *Celite 503*<sup>TM</sup> with a mean particle size of 23  $\mu$ m, (Amos et al., 2001)) in a simplified, laminar flow reactor. They showed that some 47 in every 10,000 continuous UV operations could unexpectedly fail due to random effects in UV parameters. This was despite a tolerance of 10 % over the design level of reduction in *E. coli* of  $10^{-4}$ . This meant high levels of survival of viable *E. coli* would occur each 0.58 years of continuous operation, that is, a failure on average each six calendar months in an otherwise apparently well-run and well-maintained operation. *E. coli* was chosen as the indicator micro-organism because it is a species of coliform bacteria specific to fecal material from humans and other warmblooded animals and is a widely used indicator for health risk in potable water. A drawback was the simplified nature of the laminar flow model used.

#### 4.1.1. This study

Here a Fr 13 stochastic assessment is presented for the first time of a more practical UV irradiation model with turbulent flow of water. It is based on the extensive experimental data of Ye (2007) and Ye and co-workers (2008). The aims were to demonstrate how stochastic (random) changes in UV parameters can contribute to unwanted and surprise failure of UV irradiation in an otherwise apparently well-operated and well-maintained series annular-reactor, and; to determine the likely success of proposed intervention strategies to minimize risk of failure and improve safety. Operating conditions are chosen with a view to applying findings to realistic problems related to large-scale UV irradiation for potable water production. A unit-operations model is first developed and solved using a traditional single point assessment. This is then contrasted with results from the new Fr 13 assessment. A comparison is made of results with the earlier laminar flow model of Davey and co-workers (2012). The implications of Fr 13assessments as a new quantitative tool to evaluate practical re-design and targeted physical changes to UV plant for improved safety is briefly discussed.

#### 4.2. Materials and Methods

#### 4.2.1. The annular UV reactor of Ye (2007)

The configuration of the continuous flow UV reactor of Ye (2007) and Ye and coworkers (2008) is an annular thin film in a concentric cylinder. The annular geometry is used because it is suitable for inactivating micro-organisms in for example fruit juices. A schematic is shown as Fig. 4.1. As is seen a single UV lamp sits in the central axis of the reactor. Fluid flow is in the annular gap. Depending on flow rates, flow in this gap can be turbulent or laminar. Turbulent flow is used to increase UV efficacy (Severin et al., 1984).



**Fig. 4.1:** Schematic diagram of a thin film annular-reactor between two concentric cylinders (Adapted from Ye, 2007).

A unit-operations model of UV irradiation with turbulent flow in the annularreactor can be developed as a plug flow reactor (PFR) (Levenspiel, 1999) in which firstorder kinetics for UV inactivation of *E. coli* is assumed such that:

$$\ln\left(\frac{N}{N_0}\right) = -kI_{av}\tau \tag{4.1}$$

(All symbols used are defined in the Nomenclature). The bulk residence time of the water is:

$$\tau = L/\nu \tag{4.2}$$

The average (bulk) water velocity is obtained from:

$$v = \frac{Q}{\pi \left(R_2^2 - R_1^2\right)}$$
(4.3)

Assuming the flow is uniform (steady-state), the average fluence distribution is given by (Ye, 2007):

$$I_{\rm av} = 2 \frac{\pi \int_{R_1}^{R_2} I_0 \frac{R_1}{r} \exp(-\alpha(r-R_1)) r dr}{2\pi \int_{R_2}^{R_1} r dr} = \frac{I_0 R_1 [1 - \exp(-\alpha(R_2 - R_1))]}{0.5\alpha(R_2^2 - R_1^2)} \quad (4.4)$$

Substituting for  $I_{av}$  from Eq. (4.4) into Eq. (4.1) gives:

$$\ln\left(\frac{N}{N_0}\right) = -k \frac{R_1 \left[1 - \exp\left(-\alpha (R_2 - R_1)\right)\right]}{0.5\alpha (R_2^2 - R_1^2)} I_0 \tau$$
(4.5)

If  $\alpha (R_2 - R_1) > 5$  and exp  $(-\alpha (R_2 - R_1)) << 1$ , Eq. (4.5) can be simplified to:

$$\ln\left(\frac{N}{N_0}\right) = -\frac{kI_0\tau R_c}{\alpha d}$$
(4.6)

where the gap is:

$$d = R_2 - R_1 \tag{4.7}$$

A new dimensionless group where radiation comes from the inner cylinder was defined by Ye (2007) as:

$$R_c = \frac{2R_1}{R_2 + R_1} \tag{4.8}$$

A ratio  $(c/\delta)$  is used to correct Eq. (4.6) for deviations between a real reactor and the PFR such that:

$$\ln\left(\frac{N}{N_0}\right) = -\frac{ckI_0\tau R_c}{\alpha d\delta}$$
(4.9)

For base  $log_{10}$  Eq. (4.9) is given as:

$$\log_{10}\left(\frac{N}{N_0}\right) = \ln\left(\frac{N}{N_0}\right) / 2.303 \tag{4.10}$$

The boundary layer thickness for turbulent flow  $(\delta)$  is:

$$\delta = \frac{2\mu}{\rho v f} \tag{4.11}$$

The dimensionless friction factor (*f*) is given by:

$$f = 0.079 \mathrm{Re}^{-0.25} \tag{4.12}$$

80

where the Reynolds number is:

$$\operatorname{Re} = 2d\rho v / \mu \tag{4.13}$$

Eq. (4.1) to Eq. (4.13) defines the unit-operations model for UV irradiation for potable water in turbulent flow in the annular-reactor.



Fig. 4.2: The 4-series annular-reactor of Ye (Adapted from Ye et al., 2008)

To obtain the required reduction in the number of viable *E. coli* contaminants a 4series experimental annular-reactor was used by Ye (2007) and Ye and co-workers (2008). A schematic is shown in Fig. 4.2. Each annular-reactor consisted of a single, low-pressure, germicidal UV lamp (UltraDynamics model TF-1535, Severn Trent Services Inc., Colmar, PA) surrounded by a quartz inner-cylinder and stainless steel outer-cylinder. The total irradiated length was L = 196.2 cm with a total incident fluence for the 4-lamps of  $I_0 = 55.4$  mW cm<sup>-2</sup>. The radius of the quartz inner-cylinder was  $R_1 = 1.225$  cm and the radius of the steel outer-cylinder was  $R_2 = 1.74$  cm (giving a gap of 0.515 cm). A flow rate of Q = 180 mL s<sup>-1</sup> was used to promote turbulent flow (Re > 2100). The value of the first-order UV inactivation constant for *E. coli* in water was determined (Ye, 2007) as k = 0.325 mW<sup>-1</sup> s<sup>-1</sup> cm<sup>2</sup> and the value of the coefficient for correction (Eq. (9)) c = 0.0125 cm. The value of the absorption coefficient for water from the data of Koutchma (2009) is  $\alpha = 0.01$  cm<sup>-1</sup>.

#### 4.2.2. Traditional single point simulation

Traditionally, for simulation of unit-operations in foods applications a single point, deterministic and expected value (that is, Single Value Assessment, SVA) with or without sensitivity analyses (Sinnott, 2005) is used (Davey, 2011; Davey et al., 2013). For the annular UV irradiation reactor this is done as follows: for the physical system defined by  $R_1$ ,  $R_2$ , L and Q, v = 37.5 cm s<sup>-1</sup> from Eq. (4.3). Substitution into Eq. (4.2) yields  $\tau = 5.3$  s. From, respectively, Eq. (4.7) and Eq. (4.8), d = 0.515 cm and  $R_c = 0.826$  (dimensionless). Additionally, with  $\mu = 0.93 \times 10^{-3}$  Pa.s (Ye, 2007) and, for water at 20 °C,  $\rho = 998.2$  kg m<sup>-3</sup> (Crittenden et al., 2012), Eq. (4.13) yields Re = 4148 (dimensionless). Substitution into Eq. (4.12) yields f = 0.0098 (dimensionless). Substitution for f, together with a value for the kinematic viscosity of water at 20 °C of  $v = 1.004 \times 10^{-6}$  m<sup>2</sup> s (Crittenden et al., 2012) into Eq. (4.11) gives  $\delta = 188.5$  cm.

Substitution of values for *c*, *k*,  $I_0$ ,  $\tau$ ,  $R_c$ ,  $\alpha$ , *d* and  $\delta$  into Eq. (4.9) gives a reduction in the number of viable *E. coli* of  $\ln N/N_0 = -10.02$  (dimensionless). From Eq. (4.10) the value is  $\log_{10} N/N_0 = -4.35$  (dimensionless), which is the more widely used basis for expressing reductions in viable contaminants in treated waters.

#### 4.3. Fr 13 simulation

#### 4.3.1. Defining UV failure

A fundamental requirement in Fr 13 risk assessments is a practical and unambiguous definition of failure (Davey, 2011). For the annular-reactor this will be unexpected, high levels of survival of *E. coli* post UV treatment.

A process risk factor (p) can be defined mathematically in terms of the aimed for  $log_{10}$  reduction in viable *E. coli* and the actual process reduction. For added safety, a process tolerance (*%tolerance*) can be used; the meaning of which is that the reactor should operate to give the minimum design reduction, plus an additional reduction, in viable *E. coli*. Mathematically *p* is therefore given by:

$$p = -\% \ tolerance + 100[1 - \frac{\log_{10}(\frac{\hat{N}}{N_0})}{\log_{10}(\frac{N}{N_0})}]$$
(4.14)

where 
$$\log_{10}(\frac{\hat{N}}{N_0})$$
 is an instantaneous value of  $\log_{10}(\frac{N}{N_0})$ . This form is actually

computationally convenient (Davey et al., 2013) because for all p > 0, UV irradiation fails.

#### 4.3.2. r-MC sampling

In *Fr 13* simulation the key input parameters are not defined by a point value as with traditional SVA, but by a distribution of values and the probability of each that can actually occur in practical operation. The *Fr 13* simulation output is therefore not a single value but a distribution of values with the probability of each event occurring (Davey, 2011; Davey et al., 2013). A refined Monte Carlo (r-MC) sampling is used to simulate the input parameter. This is because 'pure' Monte Carlo cannot be relied on to replicate the parameter distribution as it can both over- and under-sample from various parts of the distribution (Davey, 2010; Davey et al., 2013; Vose, 2008). The refinement is *Latin Hypercube* sampling which ensures that values are sampled from each probability distribution to cover the entire practical range. To ensure the output distribution is *Normal*, a minimum number of random samples are necessary (Vose, 2008). This is usually some 1,000 to 50,000 samples (Davey, 2011; Davey et al., 2013) (this, in any event, can be checked readily by visual inspection of the output distribution).

#### 4.3.3. Fr 13 model

Eq. (4.1) through Eq. (4.14), together with r-MC sampling of the defined probability distributions of input parameters, defines the *Fr 13* unit-operations model for UV irradiation for potable water in turbulent flow in the annular-reactor. The *Fr 13* model is therefore identical in form to the traditional model in that all mathematical operations (additions, multiplications, integrations etc.) that connect parameters are the same except that a probability distribution is used instead of a single value with error estimate (Davey, 2010; 2011; Davey et al., 2013; Sinnott, 2005). Calculations to simulate turbulent flow in the annular-reactor were carried out using Microsoft Excel<sup>TM</sup> with a commercially available add-on @*Risk*<sup>TM</sup> (pronounced atrisk) (version 5.5, Palisade Corporation). An advantage of this is that Excel has nearly universal use and thereby makes communication of results streamlined. A practical process tolerance of plus 10 % on the required  $log_{10}$  reduction of viable *E. coli* was assumed (Brigitte Carpentier, Laboratoire de securite sanitaire de Maisons-Alfort, France, *pers. comm.*).

#### 4.4. Results

Table 4.1 presents a summary comparison of results from the traditional SVA and the new *Fr 13* simulation of UV irradiation of water in turbulent flow in the annularreactor of Ye (2007) and Ye and co-workers (2008). Because the physical system has been fixed by: *c*, *L*,  $\alpha$ ,  $\mu$ ,  $\rho$ , *v*, *R*<sub>1</sub> and *R*<sub>2</sub>, the key UV operating parameters are: *I*<sub>0</sub>, *k* and *Q*. These are defined in column 1 of the table. The traditional SVA calculation, outlined above, is read down column 2 where the reduction in viable *E. coli* of 10<sup>-4.35</sup> is shown.

The *Fr 13* illustrative simulation is read down column 3 in which the UV operating parameters are reasonably assumed normal and are defined by the distribution: **RiskNormal** (mean, stdev, **RiskTruncate** (minimum, maximum)). For UV fluence the distribution used in the absence of hard commercial data is  $I_0 =$ **RiskNormal** (55.4, 5.54, **RiskTruncate** (49.86, 60.94)) to give a mean = 55.4 mW cm<sup>-2</sup> with a stdev = 10 %, and; minimum = 49.86 and maximum = 60.94 mW cm<sup>-2</sup>. This is a practical way of stating that in operation the UV lamp does vary randomly in time but that any change will not move outside this range. To acknowledge a natural biological variability in sensitivity to UV of the viable *E. coli* cells it is assumed k =**RiskNormal** (0.325, 0.0325, **RiskTruncate**  (0.2925, 0.3575)) (Amos et al., 2001). The influence of pump variation on flow of water is defined as Q =**RiskNormal** (180, 18, **RiskTruncate** (162, 198)). This flow variation of 10 % is considered usual for standard controllers (B K O'Neill, School of Chemical Engineering, The University of Adelaide, *pers. comm.*).

Ten thousand (10,000) Latin Hypercube random samples (r-MC) of each input operating parameter distribution were used to ensure a *Normally*-distributed simulation output. This means in practice that all possible combinations of process scenarios that could occur in the UV unit-operation will have been simulated.

Importantly, data shown in column 3 of Table 4.1 for *Fr 13* simulation are for one only scenario of these 10,000. A total of 1,604 failures were identified in the 10,000 scenarios, which is about 16 %. These are summarised in Fig. 4.3. The failures are seen to the right of the figure with all p > 0 and are therefore readily identified.

**Table 4.1:** Comparison of traditional single point (SVA) and *Fr 13* risk assessments for turbulent flow in 4-series annular-reactor.

Parameters	SVA*	Fr 13**	
$I_0 ({\rm mW \ cm^{-2}})$	55.4	50.4575	<b>RiskNormal</b> (55.4, 5.54, <b>RiskTruncate</b> (49.86, 60.94))
$k (\text{mW}^{-1} \text{ s}^{-1} \text{ cm}^2)$	0.325	0.3247	<b>RiskNormal</b> (0.325, 0.0325, <b>RiskTruncate</b> (0.2925, 0.3575))
$Q (\mathrm{mL s}^{-1})$	180.0	183.1978	<b>RiskNormal</b> (180, 18, <b>RiskTruncate</b> (162, 198))
$v (\text{cm s}^{-1})$	37.5	38.1841	Eq. (4.3)
$\tau$ (s)	5.3	5.1383	Eq. (4.2)
d (cm)	0.5150	0.5150	Eq. (4.7)
$R_{\rm c}$ (dimensionless)	0.8263	0.8263	Eq. (4.8)
Re (dimensionless)	4148	4221.4055	Eq. (4.13)
f (dimensionless)	0.0098	0.0098	Eq. (4.12)
$\delta$ (cm)	188.5	189.3633	Eq. (4.11)
$\ln N/N_0$ (dimensionless)	-10.02	-8.9166	Eq. (4.9)
$\log_{10} N/N_0$ (dimensionless)	-4.35	-3.87	Eq. (4.10)
p (dimensionless)		0.9810	Eq. (4.14)

\* Traditional single point, or, Single Value, Assessment

\*\* One only of 10,000 scenarios



Fig. 4.3: Distribution for the risk factor (p) for UV irradiation for potable water in turbulent flow in the 4-series annular-reactor.

Row	Volumetric flow	Incidence fluence Inactivation constant		<b>Risk factor</b>
	Q .	$I_0$	, k	р
	(mL s <sup>-1</sup> )	$(\mathbf{mW}  \mathbf{cm}^{-2})$	$({\bf mW}^{-1} {\bf s}^{-1} {\bf cm}^2)$	(dimensionless)
			-	
1	194.7383	52.0955	0.3432	0.0082
2	182.3258	54.0445	0.3037	0.2893
3	191.4998	53.6160	0.3243	0.6276
<sup>&amp;</sup> 4	183.1978	50.4575	0.3247	0.9810
5	168.4671	50.0433	0.2942	1.1751
6	182.8244	52.5624	0.3097	1.3250
7	196.9552	52.5334	0.3389	1.6494
8	190.7225	52.0797	0.3270	2.0072
9	186.3105	52.8802	0.3114	2.4112
10	185.5021	51.1656	0.3188	2.7596
11	168.5156	50.3493	0.2948	0.4675
12	194.1587	50.0273	0.3435	3.1645
13	189.2170	55.0680	0.3007	3.6106

Table 4.2: Twenty (25) selected failures from 1,604 in 10,000 UV irradiation scenarios.

14	182.8628	52.8269	0.2983	4.1905
15	191.5682	54.8932	0.3025	4.6784
16	182.5216	51.7166	0.3002	5.2695
17	168.7240	50.1579	0.2958	0.6523
18	185.9576	52.1671	0.3025	5.8501
19	189.8552	54.4526	0.2954	6.4244
20	194.6565	50.4537	0.3266	7.0169
21	196.1355	56.1733	0.2927	7.9741
22	182.4156	50.6671	0.2927	8.9987
23	168.8120	50.0162	0.2986	0.1102
24	188.5492	49.9029	0.3032	10.6892
25	169.9687	51.0380	0.2927	0.8788

<sup>&</sup> particular scenario of Table 4.1.

#### 4.5. Discussion

#### 4.5.1 Fr 13 failures

To highlight how these failures actually arise in practice, 25 were randomly selected and are presented as Table 4.2. A practical advantage of the data in this table is that the particular combination of UV parameters that resulted in the failure can be easily identified. An example in bold print (row 4 of the table), shows the particular combination of randomly sampled values for Q = 183.2 mL s<sup>-1</sup>,  $I_0 = 50.46$  mW cm<sup>-2</sup>, and; k = 0.3247 mW<sup>-1</sup> s<sup>-1</sup> cm<sup>2</sup>, resulted in greater survival of *E. coli* than designed and therefore failure to produce potable water. This is underscored by the corresponding value of the risk factor of p = 0.981 and, is the particular scenario presented in Table 4.1. It is interesting to note that for this combination Q is greater than the mean,  $I_0$  less than the mean and k very nearly equal to the mean, of the practical distributions used to define the parameters.

Other combinations of parameters can be readily identified in the table, for example, row 25 in which Q is less than the mean, indicating a longer residence time of the
water in the annular-reactor and the potential for reduced survival of *E. coli* therefore; but it is seen the chance corresponding values of UV fluence ( $I_0$ ), and inactivation constant (k) for viable *E. coli*, are also less than the mean values of the distribution. This chance combination of process parameters results in UV failure (p = 0.8788). In summary, a detailed study of all 1,604 combinations of the three UV process parameters that resulted in p > 0 underscores that the UV success or failure cannot be readily intuitively 'guessed' directly from parameter values.

Clearly, the greater the number of process parameters in a unit-operation the more difficult it becomes to intuit success or failure of the operation based on a sound knowledge of the particular values of process parameters. This fact underscores the elegant utility of the risk factor, especially with increasing complexity in any unit-operation.

#### 4.5.2 Visualizing Fr 13 risk

Although the tabulated data of Table 4.2 do give a practical insight into UV operation, a difficulty is to gain an immediate overall perspective, or visualisation, of p values that actually underscore UV failure for potable water. To try to achieve this, a 3D plot of the 25 selected values from Table 4.2 was produced using commercially available software (Statistica<sup>TM</sup> version 10, StatSoft Inc.) and is presented as Fig. 4.4. Part a) of this figure shows a scatter plot for the three UV parameters, respectively, Q,  $I_0$  and k. The plot in part b) shows the surface plot for all 25 values p > 0. The random nature of the p values in time with continuous operation means that the surface plot cannot be extrapolated in any reliable way. It does serve to show however that at the values of Q greater than the mean (> 180 mL s<sup>-1</sup>) UV is increasingly likely to fail with the unwanted survival of viable E. *coli*. Whilst this graphical treatment seems to work for the three praameter unit-operation

model for this study, a radar plot could be more useful with increased numbers of key parameters in increasingly sophisticated process models (K R Davey, *unpublished data*).



**Fig. 4.4:** Plot of the 25 selected *Fr 13* failures (p > 0) of Table 4.2: 3D scatter plot (a) and 3D surface plot (b).

Importantly, the new *Fr 13* risk simulation reveals that, on average, viable *E. coli* will unexpectedly survive UV treatment in greater number in the series annular-reactor in about 16 % of all continuous operations over the long term, that is, 1,604 in each 10,000 due to stochastic effects within the physical system of the unit-operation. This will be despite apparent best operation and maintenance. If each simulation is considered an operating day, with prolonged periods of operation, this is translated as 1.92 (=  $1,604/10,000 \times 12$ ) surprise (unexpected) failures each calendar month. However, it cannot be assumed these will actually be spaced evenly in time. Importantly this new insight is not provided by alternative current risk methodology, with or without sensitivity analyses.

A *Fr* 13 simulation can be thought of as a kind of extended risk sensitivity analysis of how often the UV could probably failed. This is because all combinations of parameters that could actually occur in practical operations are considered and quantified.

#### 4.5.3 Input probability distributions for Fr 13

An important consideration that arises with the carrying out any Fr 13 risk assessment is how the value of the risk factor (p), and therefore the predicted surprise failure frequency, will be impacted by the probability distribution used to define the key operating parameters. Clearly, the more realistic the input probability distribution used for key parameters, the better the simulation for Fr 13 failure. In general, the most realistic simulations will made with hard data, or expert knowledge. These aspects have been discussed earlier (Davey, 2010; Davey et al., 2013); to summarize, there are in principal some 40 distribution types (Vose, 2008) that might be used, including: *Triangle, Beta Subjective, Tnormal* (e.g. Cerf and Davey, 2001; Davey and Cerf, 2003) and Normal (Davey et al., 2013; Davey, 2011; Patil et al., 2005), all with or without truncations (Davey, 2011).

Truncation is an important characteristic. From a practical point of view for example, were a *Normal* probability distribution used, for say, atmospheric pressure (mm Hg) the probability of atmospheric pressure being near zero, or 1,000 (mmHg) in any fixed global location is small. Rather, there will be a practical range that simulates the experienced atmospheric pressures over a long period, so the distribution must be realistically truncated to reflect this, say 720 (minimum) to 790 (maximum), mmHg.

In this study, in the absence of alternate data, the 1 x stdev assumed about the mean with the **RiskNormal** distributions for all three key UV parameters,  $I_0$ , k and Q, means that 2/3 (68.2 %) of all r-MC values sampled will fall in this interval (Sullivan, 2004). The distributions used have also been truncated (*minimum* = mean – 1 x stdev, *maximum* = mean + 1 x stdev) to approximate the most practical set of realistic values and outcomes for p.

With the **RiskNormal** distribution, a 3 x stdev will mean nearly all r-MC samples (99.7 %) will fall in this interval (Sullivan, 2004). Repeat simulations were carried to test the impact of an increased variance of 3 x stdev about the **RiskNormal** mean and **RiskTruncate** (*minimum* and *maximum*) in each of the three key parameters,  $I_0$ , k and Q of the *Fr* 13 unit-operations model for UV irradiation for potable water. For example for  $I_0$ , the input probability distribution becomes **RiskNormal** (55.4, 16.62, **RiskTruncate** (38.78, 72.02). Results show that the impact is to give a failure rate of 13 %. This is not considered meaningfully different from that of 16 % (1 x stdev).

Some experimenting will generally show that the failure frequency is not highly sensitive to a range of distributions (K R Davey, *unpublished data*). A *Normal* distribution

is however readily justified in the absence of contrary hard data or theoretical considerations.

The overriding criterion in selection of the probability distribution however is that each scenario outcome produced must be practically observable in real operation; the chance (probability) of each actually occurring is taken-care of in the distribution.

#### 4.5.4 Minimizing Fr 13 risk

Because Fr 13 surprise failure is due solely to stochastic (chance) effects, more study or measurement cannot be used to reduce this type of vulnerability of the unitoperation. However, this situation actually leads to a very practical application of the Fr 13method for improving design and safety. This is simulation in second-tier studies (Davey, 2010; 2011; Davey et al., 2013) where Fr 13 failure can be minimized through proposed physical re-designs of the operation or through changes to variance in the key input parameters. This is illustrated in what follows.

For the annular UV irradiation reactor three options for improved safety and reduced vulnerability to  $Fr \ 13$  risk are apparent. The first is to specify an increase in the safety tolerance. Repeat simulations are summarized in Fig. 4.5 for a range from 5 % to 30 %. It is seen that the number of  $Fr \ 13$  failures, expectedly, falls away with increased tolerance and rises sharply with reduced tolerance. There is an apparent exponential dependence on failure rate with tolerance. The figure shows however the practical limit is about 30 % after which no reduction in the number of  $Fr \ 13$  failures is obtained.



**Fig. 4.5:** Effect of *%tolerance* on  $\log_{10}$  reduction in viable *E. coli* against the number of *Fr 13* failures per 10,000 scenarios of continuous UV irradiation for potable water in the 4-series annular-reactor.

A second is to reduce the variance on the continuous flow rate of water through the reactor (Q). In practice this means a much-improved flow controller. Repeat simulations are presented in Fig. 4.6 for a range of values of the parameter distribution with a stdev of 2, 5, 8 and 10 %. The number of failure is seen to rise with increased stdev and fall away as stdev is decreased. This suggests that increased costs for improved process control with small fluctuations (low stdev) in water flows might be readily justified.



**Fig. 4.6:** Effect of variability (%-stdev) on the volumetric flow rate ( $Q = 180 \text{ mL s}^{-1}$ ) against the number of *Fr 13* failures in UV irradiation for potable water in the 4-series annular-reactor.

A third is to reduce any variance on UV fluence ( $I_0$ ), that is, to improve the quality of the UV lamp. UV lamps do age with time (Bolton and Cotton, 2008). Repeat simulations show that a halving of the variance on fluence will reduce vulnerability of *Fr 13* failures from 1,604 to 1,370. The cost of the UV lamp may increase significantly to achieve this.

Significantly however, from a practical view, it is not possible to reduce the susceptibility to UV irradiation of *E. coli* because of natural micro-biological variability, and therefore no changes to the inactivation constant (k) can be purposely made in a physical re-design of the unit-operation.

A comparison can be made of results for the turbulent flow annular-reactor of Ye (2007) with those of the laminar flow reactor of Davey and co-workers (2012). A comparative summary is given as Table 4.3.

Table 4.3: Comparison of Model I (laminar flow reactor of Davey and co-workers (2012))
with Model II (turbulent flow annular-reactor of Ye (2007) and Ye and co-workers
(2008)) for UV irradiation of *E. coli* for potable water.

Parameter	Model IModel II(simplified laminar flow)(4-series annular-reactor)	
Reactor flow regime	Laminar	Turbulent
Fluence, $I_0$ (mW cm <sup>-2</sup> )	11.9	55.4
Residence time, $\tau$ (s)	1.90	5.22
First-order UV inactivation constant, $k$ (mW <sup>-1</sup> s <sup>-1</sup> cm <sup>2</sup> )	0. 414	0. 325
$\log_{10} (N/N_0)$ , (dimensionless)	- 4.08	- 4.35
<i>Fr 13</i> failures, (%)	0.4	16
Description	Too simplified (?), but includes suspended solids	Sophisticated analysis, involves absorption properties, no suspended solids

**Model I** shown in the table is the laminar-flow UV model (Davey et al., 2012) and **Model II** is the turbulent flow model of Ye (2007) and Ye and co-workers (2008) used in the present study. Both models achieve the same design reduction in viable *E. coli* of ~  $10^{-4}$ . An apparent contrast is the greater vulnerability to *Fr 13* failure in continuous operation of 16 % with **Model II** compared to 0.4 % for **Model I**. However, caution is needed as it is difficult to actually compare directly the difference between the two models since both have different parameters, for example **Model I** includes UV-shielding suspended solids while **Model II** includes absorption coefficient. However, overall it is satisfying that the first-order inactivation kinetics for both is similar (for **Model I** is  $k = 0.4139 \text{ mW}^{-1} \text{ s}^{-1} \text{ cm}^2$  and  $k = 0.325 \text{ mW}^{-1} \text{ s}^{-1} \text{ cm}^2$  for **Model II**).

Because a relatively high flow rate is required to sustain turbulent flow with **Modell II**, a 4-series reactor was necessary to give the needed residence time ( $\tau = 5.22$  s). Useful further direct contrast is limited because the two assessments involve different defined parameter distributions ( $I_0$ , Q and k for **Model II**;  $I_0$ ,  $\tau$  and concentration of UV-shielding material for **Model I**). Further simulations might be made, however the more realistic **Model II** could now be extended to include effects of both UV-shielding and UV-absorbing suspended solids using, for example, the published experimental data of Amos and co-workers (2001). The concentrations of both these effects on UV could be defined to usefully and more realistically simulate water quality and flows and fluctuations for particular geographical sites or industries.

Other contaminant water micro-organisms could also be incorporated, especially *Giardia* (Linden et al., 2002). *Giardia* is a prevalent and relatively resistant water pollutant that can be treated with UV irradiation (Gibson et al., 1999; Linden et al., 2002).

#### 4.5.6 Coupling Fr 13 with commercial technologies

The valuable insight to be gained with Fr 13 risk modelling over traditional methods is to quantitatively identify all process scenarios that are probable, including surprise failures.

The fact that the *Fr* 13 risk modelling is predicated on universal unit-operations principles has led to hypotheses that it could be coupled with commercial technologies, such as Aspen Plus® or Batch Process Developer®, to produce significantly more powerful process design and assessment tools than are currently available (Davey, 2010).

#### 4.6. Conclusions

A new *Fr 13* risk analysis of turbulent flow UV irradiation for potable water in the annular-reactor of Ye (2007) and Ye and co-workers (2008) has highlighted that failure, defined by unexpected survival of viable *E. coli* post-treatment, can result from random (stochastic) effects in prolonged continuous operation.

The number of failures is related to the combined effects of variance about process parameter mean values. This means that continuous operation is actually a mix of successful and failed states, and neither 'human error' nor 'faulty fittings' (Davey, 2011) need to be invoked as an explanation. Importantly these Fr 13 insights are not available from current risk analyses. Reducing the variance in key parameters, through for example improved process control, whilst potentially costly, can minimize likelihood of UV failures.

 $Fr \ 13$  failure assessments can be used in second-tier studies to quantitatively assess risk from proposed changes in control or design and intervention strategies, and therefore can be used to guide improvements to better process safety and equipment.

## Nomenclature

The number in parentheses after description is the equation in which the symbol is defined or first used.

С	correction constant for real reactor, cm (4.9)
d	annular gap width, cm (4.9)
f	friction factor, dimensionless (4.11) and (4.12)
I <sub>av</sub>	average fluence of ideal plug flow reactor, mW cm <sup>-1</sup> (4.1)
$I_0$	incident fluence, mW cm <sup><math>-2</math></sup> (4.6) and (4.9)
k	inactivation constant, $mW^{-1} s^{-1} cm^2 (4.1)$ , (4.6) and (4.9)
L	length of radiation section, $cm (4.2)$
Ν	concentration viable <i>E. coli</i> , $mL^{-1}(4.9)$ and $(4.10)$
$N_0$	concentration viable <i>E. coli</i> before UV exposure, $mL^{-1}$ (4.9) and (4.10)
p	risk factor, dimensionless (4.14)
Q	volumetric flow rate, mL s <sup><math>-1</math></sup> (4.3)
$R_1$	radius of inner cylinder, cm (4.3), (4.7) and (4.8)
$R_2$	radius of outer cylinder, cm (4.3), (4.7) and (4.8)
R <sub>c</sub>	dimensionless group (4.8)
Re	Reynolds number, dimensionless (4.13)
v	average water velocity in annular gap, cm $s^{-1}$ (4.3)

## Greek symbols

α	absorption coefficient, $\text{cm}^{-1}(4.6)$ and (4.9)
$\delta$	boundary layer thickness, cm $(4.9)$ and $(4.11)$
μ	dynamic viscosity of water, 0.93 x $10^{-3}$ Pa. s (4.11) and (4.13)
ρ	density of water at 20 $^{\circ}$ C, 998.207 kg m <sup>-3</sup> (4.13)
τ	average residence time, s $(4.1)$ and $(4.2)$
υ	kinematic viscosity of water at 20 $^{\circ}$ C, 1.004 x 10 $^{-6}$ m <sup>2</sup> s (4.11)

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# IMPACT OF SUSPENDED SOLIDS ON FR 13 FAILURE OF UV IRRADIATION FOR INACTIVATION OF ESCHERICHIA COLI IN POTABLE WATER PRODUCTION WITH TURBULENT FLOW IN AN ANNULAR REACTOR

# IMPACT OF SUSPENDED SOLIDS ON *FR 13* FAILURE OF UV IRRADIATION FOR INACTIVATION OF *ESCHERICHIA COLI* IN POTABLE WATER PRODUCTION WITH TURBULENT FLOW IN AN ANNULAR REACTOR

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- the candidate's stated contribution to the publication is accurate (as detailed above);
- ii. permission is granted for the candidate in include the publication in the thesis; and

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#### Abstract

Ultraviolet irradiation (UV) is an important alternative to disinfection for production of potable water. Viable *Escherichia coli* is a widely used indicator for public health risk. However, UV efficacy is reduced by suspended solids that can act as both UV shielding and UV absorbing, agents. Failure of UV irradiation can lead to an enduring health legacy. Here the probabilistic Fr 13 methodology of Davey and co-workers (Chem. Eng. Sci., 126 (2015) 106 – 115) is demonstrated for turbulent flow of feed water with suspended solids irradiated in an annular reactor and, a comparison made with the traditional deterministic method. The aim was to examine the impact of naturally occurring fluctuations in suspended solids concentration on failure to inactivate viable E. coli. A UV failure factor (p) is defined in terms of the design and actual  $\log_{10}$  reduction in viable E. coli. UV irradiation is simulated using (Latin Hypercube) Monte Carlo sampling. Illustrative overall results show some 32.1 % and 43.7 % of apparent successful operations could unexpectedly fail over the long term due, respectively, to combined impact of random fluctuations in feed water flow (Q), lamp intensity ( $I_0$ ) and shielding and absorption of UV by suspended solids [conc]. This translates to four (4) failures each calendar month (the comparison rate without suspended solids is 16 % or two (2) failures per month). An unexpected finding however is, although the initial presence of suspended solids as both UV shielding (median particle size 23 µm) and absorbing agent has a highly significant impact on reducing UV efficacy, fluctuations in concentration of these in the feed water do not meaningfully impact overall vulnerability. UV failure is impacted highly significantly by fluctuation in feed water flow. It is concluded this is strong quantitative evidence to emphasize that solids should be removed prior to the UV reactor, and that an improved flow control be used to reduce variance on feed water flow, rather than increased UV dose.

This work will be of benefit to operators of UV equipment and researchers in risk analyses.

### Keywords:

ultraviolet irradiation for potable water; UV risk analysis; UV efficacy with suspended solids; failure of UV irradiation; Friday 13th risk modelling; *Fr 13* risk

## Highlights

- UV efficacy for potable water significantly impacted by initial suspended solids
- However UV efficacy not vulnerable to fluctuations in suspended solids
- Overall UV efficacy is a mix of successful and unsuccessful inactivation of E. coli
- Results can be used to improve UV efficacy, reliability and safety
- Benefit to designers, operators and risk analysts of UV treatment for potable water

#### 5.1. Introduction

Ultraviolet irradiation (UV) is a practical alternative to halogen disinfection e.g. chlorine for production of potable water (Bilton, 2010; Amos et al., 2001; Das, 2001). The post-treatment presence of viable *Escherichia coli*, a pathogenic contaminant, is widely used as an indicator of efficacy of potable water production and health risk (Stevens et al., 2003; Loge et al., 1999). Failure of UV irradiation to reduce these viable pathogens to a safe level can lead to an enduring public health legacy.

A reliable and quantitative understanding of risk of UV irradiation for potable water is therefore important.

An emerging risk methodology is that of Davey and co-workers. Their thesis is that naturally occurring, chance fluctuations in otherwise well-operated plant parameters can accumulate in one-direction and lead unexpectedly to surprise (sudden) failure in either process or product about a binary divide. They called this *Fr 13* (Friday 13<sup>th</sup>) failure to underscore the nature of the occurrence. Published studies include surprise failure of a large-scale, coal-fired-boiler from thermally efficient to inefficient (Davey, 2015), pasteurization failure of raw milk to meet regulatory standards (Chandrakash et al., 2015), failure of Clean-In-Place from successful removal of whey protein deposits to failure to remove these (Davey et al., 2015; 2013; Chandrakash, 2012), failure in continuous UV irradiation from potable to non-potable water (Abdul-Halim and Davey, 2015; Davey et al., 2012), from stable fermentation to un-stable (washout) (Patil, 2006; Patil et al., 2005), failure of batch-continuous UHT milk from sterile to non-sterile (Davey and Cerf, 2003; Cerf and Davey, 2001), and; more generally, from safe to unsafe operation (Davey, 2011; Nolan and Barton, 1987). Overall, this work shows that without breakage, shutdown or

faulty fittings, well-operated and well-maintained continuous operations can in fact be an instantaneous mix of successful and failed operations (Davey, 2015; Gujer, 2008).

A practical advantage claimed for Fr 13 is that all process scenarios that could exist can be quantified, including failures. It is claimed to be more mathematically correct than alternate risk and hazard methods because knowledge about the process is separated from impact of random fluctuation in parameters (Abdul-Halim and Davey, 2015; Davey et al., 2015; Rai and Krewski, 1998; Hoffman and Hammonds, 1994). It therefore has the advantage that it permits the effect of each to be studied (Davey, 2015).

The possible risk with fluctuation in parameters about a steady-value is the focus of recent approaches of Aven (2010) and Haimes (2009), and Milazzo and Aven (2012). A key drawback however is that these approaches remain largely qualitative, and are not rigorously quantitative.

Importantly, *Fr 13* is based on established unit-operations (Foust et al., 1980; Wankat, 2007; McCabe et al., 2001) and not subjective or qualitative views of 'credible' risk scenarios as with this approach, and others, for example, HAZOP and HACCP.

As highlighted in the Blackett review (Anon., 2012) low probability, high impact failures are a major theoretical and practical concern for companies and governments of almost every size. In potable water production these failures are acknowledged as real events and can have a significant 'snow-ball' effect in determining the end quality of integrated processes. Remarkably, *Fr 13* event is a notion that has long persisted in the industrial West (Suddath, 2009).

An initial *Fr 13* assessment of UV irradiation was presented by Davey et al. (2012) for a simplified, laminar flow reactor with *E. coli* as contaminant. Results revealed that 0.4 % of UV operations over the long term could unexpectedly fail due to the accumulated impact of naturally occurring random fluctuations in UV intensity and residence

(treatment) time. A drawback however was the simplified nature of the laminar model used. To overcome this, an improved UV irradiation model was synthesised by Abdul-Halim and Davey (2015) for more usual turbulent flow in an annular reactor based on the work of Ye (2007). Results showed 16 % of apparent successful operations, over the long term, could fail to achieve the Regulatory (Anon., 2013; Sommer et al., 2008) design reduction in viable *E. coli*  $\ge 10^{-4}$  due to the impact of random effects.

It is widely known however that UV efficacy is reduced by the presence of suspended solids as these can both absorb UV light and shield contaminants from UV (Cantwell and Hoffman, 2011; Winward et al., 2008; Amos et al., 2001; Emerick et al., 2000; Loge et al., 1999; Parker and Darby, 1995). There is a need therefore for a quantitative risk assessment of the impact of suspended solids on UV irradiation efficacy and possible UV failure for potable water production with turbulent flow.

#### 5.1.1. Purpose of this study

Here, we extend the work of Abdul-Halim and Davey (2015) to quantitatively assess the impact of naturally occurring random fluctuations in concentration of suspended solids on vulnerability to  $Fr \ 13$  failure of UV irradiation for potable water production. *E. coli* is used as the indicator pathogen. The aim was to quantitatively investigate the impact of accumulated naturally occurring chance fluctuations in the concentration of suspended solids, together with those in UV lamp intensity and feed water flow on inactivation of *E. coli*.

A unit-operations model incorporating suspended solids, as both shielding and absorbing agents, on UV inactivation of *E. coli* based on published work is synthesised and solved using traditional, deterministic methods. Findings are contrasted with the new

Fr 13 methodology. Results are compared with previous findings and used to assess practical re-design to minimize vulnerability to Fr 13 failure of UV irradiation of water with suspended solids present.

A justification for this work is that incorporation of, and knowledge about, the impact of suspended solids will lead to improved and more realistic simulations and therefore improved UV designs, reliability and safety.

#### 5.2. Materials and methods

#### 5.2.1. UV inactivation of E.coli with suspended solids present

Amos et al. (2001) presented extensive experimental data (n = 40) and analyses for UV inactivation of *E. coli* ATCC 25922 (FDA strain, Seattle 1946) in the presence of suspended solids, and the development and assessment of four predictive model forms. Experimental work was carried out in a commercial UV Unit (Model LC-5, Ultraviolet Technology Australasia Pty Ltd, Australia). The suspended solids used to alter the (reverse osmosis) water transmittance were diatomaceous earth (as *Celite 503*<sup>TM</sup>) for controlled UV shielding (89 % SiO<sub>2</sub> with median particle size 23 µm), and coffee powder (International Roast<sup>TM</sup>) for controlled UV absorbing. Model forms evaluated included classical loglinear, Davey linear-Arrhenius (DL-A) (Ross and Dalgaard, 2004; McMeekin et al., 1993; Davey, 1993), square-root (i.e. Ratkowsky-Belehradek) (Ratkowsky, 1990; Belehradek, 1926) and a third-order polynomial (*n*OP). Test criteria for model rankings were based on the goodness of fit (percent variance accounted for (%V) (Snedecor and Cochran, 1989), relative complexity (i.e. parsimony) (McMeekin et al., 1993; Davey, 1993), ease of synthesis and use, and; potential for physiological interpretation of coefficients. The DL-A was found to best explain the data (% V = 97.2) and overall best fulfilled the test criteria for a predictive model for inactivation with both UV shielding and UV absorbing from suspended solids. The model form is given by

$$\ln k = C_0 + C_1 [dose] + C_2 [dose]^2 + C_3 [conc]$$
(5.1)

where UV dose is

$$[dose] = I_0 \tau \tag{5.2}$$

and  $k = \mu W^{-1} s^{-1} cm^2$ . All symbols used are carefully defined in the Nomenclature. The model is applicable to a range of concentration of shielding agent  $0.01 \le [conc] \le 0.3$ , g L<sup>-1</sup> and absorbing agent  $0.001 \le [conc] \le 0.03$ , g L<sup>-1</sup>.

The model form is said to be linear-Arrhenius and 'additive' (Ross and Dalgaard, 2004; Davey, 1993; Amos et al., 2001). The values for the model coefficients ( $C_0 - C_3$ ) are presented in Table 5.1 for UV inactivation of viable *E. coli* in the presence of both UV shielding and UV absorbing agents.

**Table 5.1:** Coefficients for the Davey linear-Arrhenius (DL-A) model for UV irradiation inactivation of viable *E. coli in* the presence of suspended solids as both UV shielding and UV absorbing agents

$$\ln k = C_0 + C_1 [dose] + C_2 [dose]^2 + C_3 [conc]$$

with k in  $\mu W^{-1} s^{-1} cm^2$  for a range of concentration of shielding agent  $0.01 \le [conc] \le 0.3$ , g L<sup>-1</sup> and absorbing agent  $0.001 \le [conc] \le 0.03$ , g L<sup>-1</sup>.

UV agent	$C_0$	C <sub>1</sub> x 10 <sup>-4</sup>	C <sub>2</sub> x 10 <sup>-9</sup>	<i>C</i> <sub>3</sub>
Shielding	- 6.344	- 0.771	0.723	- 0.685
Absorbing	- 5.866	- 1.14	1.30	- 11.04

#### 5.2.2. An annular UV reactor unit-operations with turbulent flow

The unit-operations annular reactor of Abdul-Halim and Davey (2015) was based on the experimental work of Ye (2007) who used a single, low-pressure UV lamp surrounded by a quartz inner-cylinder and stainless steel outer-cylinder. The quartz innercylinder radius was  $R_1 = 1.225$  cm and the steel outer-cylinder radius  $R_2 = 1.74$  cm (creating a gap, d = 0.515 cm). The irradiated (4-series) length was L = 196.2 cm. For turbulent flow (Re > 2,100), the water flow rate is Q > 180 mL s<sup>-1</sup>.

The unit-operations model presented by Abdul-Halim and Davey (2015) for turbulent flow in the annular-reactor was a plug-flow reactor (PFR) such that

$$\ln\left(\frac{N}{N_0}\right) = -\frac{ckI_0\tau R_c}{\alpha d\delta}$$
(5.3)

For a more convenient  $log_{10}$  base, Eq. (5.3) was written

$$\log_{10}\left(\frac{N}{N_0}\right) = \ln\left(\frac{N}{N_0}\right)/2.303 \tag{5.4}$$

The residence time of the water in the reactor was given by

$$\tau = L/v \tag{5.5}$$

The water velocity in the gap is

$$v = \frac{Q}{\pi \left(R_2^2 - R_1^2\right)}$$
(5.6)

A dimensionless group for radiation from the inner cylinder defined by Ye (2007) is

$$R_{c} = \frac{2R_{1}}{R_{2} + R_{1}} \tag{5.7}$$

The annular gap dimension is

$$d = R_2 - R_1 \tag{5.8}$$

The ratio  $(c/\delta)$  was used by Ye (2007) to correct for deviation of a real reactor from a PFR. The boundary layer for turbulent flow  $(\delta)$  is

$$\delta = \frac{2\mu}{\rho v f} \tag{5.9}$$

The friction factor (f) is

$$f = 0.079 \mathrm{Re}^{-0.25} \tag{5.10}$$

Where

$$Re = 2d\rho v / \mu \ge 2,100 \tag{5.11}$$

in which 2*d* is the hydraulic diameter for the annulus (outer – inner, cylinder diameter). The transition from laminar to turbulent flow occurs when  $2,100 \le \text{Re} \le 4,000$  and a fully developed turbulent flow when  $\text{Re} \ge 4000$  (Koutchma et al., 2009).

Eq. (5.1) through to Eq. (5.11) defines UV irradiation for inactivation of viable *E*. *coli* for potable water in the presence of suspended solids in turbulent flow in the annular reactor of Ye (2007). For Eq. (5.3), c = 0.0125 cm (Ye, 2007).

Importantly, Eqs. (5.3) and (5.4), show predicted log reductions in *E. coli* decrease with an increase in  $\alpha$  in this reactor. This is because influence decreased exponentially with path length from the UV radiation source i.e. 'small increases in  $\alpha$  resulted in large increases in under-irradiated volumes' (Ye, 2007). This was successfully experimentally demonstrated by Ye (2007) for this reactor (who concluded that a thin (much less than the d = 0.515 cm) gap would need to be used for juices which have high values of  $\alpha$ ).

A value of the absorption coefficient  $\alpha = 0.01 \text{ cm}^{-1}$  was used for UV treatment of the clean water of Abdul-Halim and Davey (2015), here however for contaminated water with suspended solids, this is assumed to be  $\alpha = 0.0055 \text{ cm}^{-1}$  (Vasiliev and Alameh, 2008).

#### 5.2.3. Traditional single value assessment (SVA) simulation

Typically, in the water and food industries, unit-operations models are solved using a traditional, deterministic single point value, or single value assessment (SVA). This can be done with or without sensitivity analyses (Sinnott, 2005).

For the turbulent flow annular UV reactor defined by  $I_0 = 55,400 \ \mu\text{W cm}^{-2}$ ,  $Q = 500 \ \text{mL s}^{-1}$ ,  $L = 196.2 \ \text{cm}$ ,  $R_1 = 1.225 \ \text{cm}$  and  $R_2 = 1.74 \ \text{cm}$ , and for the inactivation of viable *E. coli* defined by the model coefficients for UV shielding of Table 5.1, this is carried out as follows: from Eq. (5.6)  $v = 104.22 \ \text{cm s}^{-1}$ ;  $\tau = 1.9 \ \text{s}$  from Eq. (5.5), and;  $[dose] = 104,298 \ \mu\text{W} \ \text{s} \ \text{cm}^{-2}$  from Eq. (5.2). From Eq. (5.1) (Table 5.1) at a mid-range value  $[conc] = 0.115 \ \text{g} \ \text{L}^{-1}$ ,  $k = 0.00136 \ \mu\text{W}^{-1} \ \text{s}^{-1} \ \text{cm}^2$ . Eq. (5.7) and Eq. (5.8) respectively yield  $R_c = 0.8263$  (dimensionless) and  $d = 0.515 \ \text{cm}$ . Given  $\mu = 0.93 \ \text{x} \ 10^{-3} \ \text{kg} \ \text{m}^{-1} \ \text{s}^{-1}$  (Ye, 2007) and, for water (20 °C)  $\rho = 998.2 \ \text{kg} \ \text{m}^{-3}$  (Crittenden et al., 2012), Eq. (5.11) yields Re = 11,521 (dimensionless). From Eq. (5.10) f = 0.0076 (dimensionless). The value of the kinematic viscosity of water (20 °C) used is  $v = 1.004 \ \text{x} \ 10^{-6} \ \text{m}^2 \ \text{s}^{-1}$  (Crittenden et al.,

2012). Substitution together with the value for *f* into Eq. (5.9) gives  $\delta = 243.39$  cm. The reduction in the number of viable *E. coli* is computed from substitution of values for *c*, *k*,  $I_0$ ,  $\tau$ ,  $R_c$ ,  $\alpha$ , *d* and  $\delta$  into Eq. (5.3) to give  $\ln N/N_0 = -2.13$  (dimensionless). From Eq. (5.4) therefore  $\log_{10} N/N_0 = -0.92$  (dimensionless).

Based on these experimental data of Amos et al. (2001) this is notably a highly significant reduction in UV efficacy in the annular reactor from the  $log_{10} = 4.35$  reported by Abdul-Halim and Davey (2015) due to the presence of UV shielding agent.

Similarly, for the presence of UV absorbing solids it can be shown,  $\log_{10} N/N_0 = -$  0.99.

#### 5.2.4. Fr 13 model and simulation

Failure of UV was defined by Abdul-Halim and Davey (2015) using a convenient dimensionless coefficient given by

$$p = -\% tolerance + 100[1 - \frac{\log_{10}(\frac{N}{N_0})}{\log_{10}(\frac{N}{N_0})}]$$
(5.12)

where  $\log_{10}(\frac{\hat{N}}{N_0})$  is an instantaneous value of  $\log_{10}(\frac{N}{N_0})$  (or more mathematically correct,

one possible scenario).

Eq. (5.12) is convenient because for all p > 0, UV irradiation will have failed. A practical process tolerance (margin) of plus 10 % on the required  $\log_{10}$  reduction of viable *E. coli* was assumed by Abdul-Halim and Davey (2015) i.e. if the design  $\log_{10}$  reduction in viable *E. coli* plus 10 % is not achieved, the UV treatment was said to have failed.

The *Fr 13* failure model for UV irradiation of viable *E. coli* for potable water production with turbulent flow in the presence of suspended solids in an annular reactor is given by Eq. (5.1) through Eq. (5.12).

In *Fr 13* simulations, the key parameters are defined by probability distributions and not by single, 'best guess' values. These probability distributions are used to imitate the naturally occurring fluctuations in parameter values in time (Davey et al., 2015; Davey, 2011; Tucker et al., 2003; Vose, 1998). In the absence of unconditional (hard) data, normal distributions, which are truncated so as to obviate nonsensical values of the key parameters, have been used (e.g. Davey, 2015; Davey et al., 2015; Chandrakash, 2012; Davey, 2011; Patil, 2006; Patil et al., 2005). However, other types of distributions might be more suited if there are conditional data. For example, Davey and Cerf (2003) used a **BetaSubjective** distribution (Vose, 2008) to imitate residence time in a UHT milk plant, and a Triangle distribution (Vose, 2008) to imitate the decimal reduction time of viable populations of *Bacillus stearothermophilus* and *Bacillus thermodurans*. There are some 40 distribution types (Vose, 1998).

A refined Monte Carlo with a Latin Hypercube sampling (r-MC) is used to ensure values are sampled that cover the entire range of the distribution. (Sampling with 'pure' MC for e.g. cannot be relied on to replicate the distribution because it can both over- and under-sample from various parts of the distribution). If the number of samples is sufficiently large, the output mean of a product of a large number of independent positive parameters that have different distribution functions will be approximately normally distributed (Vose, 2008). Davey and co-workers (e.g. Abdul-Halim and Davey, 2015; Davey et al., 2015; 2013; Davey, 2011) have reported that this is usually some 1,000 to 50,000 samples for typical unit-operations simulations. (The number is readily established when a plot of number of failures, all p > 0, versus number of r-MC samples has plateaued

to a constant value). Importantly with a sufficiently large number of r-MC samples, all possible combinations of input parameter values and resulting output process scenarios that could occur in practical UV irradiations with suspended solids present will have been simulated, including failures.

The  $Fr \ 13$  model is seen therefore to be identical to the traditional one in which all mathematical operations, additions, multiplications etc., that join parameters are the same, but one in which parameters are defined by distributions of values and not by single values (with error estimate); clearly therefore the  $Fr \ 13$  output will be a distribution.

Simulations were carried out using Microsoft Excel<sup>™</sup> with commercially available add-on @*Risk*<sup>™</sup> (version 5.5, Palisade Corporation). Excel spread sheeting is advantageous as it has nearly universal use making communication of results straightforward. Additionally, the distributions defining naturally occurring fluctuations in parameters can be entered, viewed, copied and pasted and manipulated as Excel formulae. Ten thousand (10,000) samples were found sufficient.

#### 5.3. Results

Table 5.2 presents a comparison and summary of the traditional SVA with the new *Fr 13* simulation of UV irradiation of viable *E. coli* for potable water with DL-A inactivation kinetics in the presence of UV shielding agent. UV key parameters are defined in column 1 of the table. The traditional SVA calculations are presented and read down column 2 where it is seen about  $1-\log_{10}$  reduction (i.e. - 0.92) in viable *E. coli* is obtained.

The *Fr 13* simulation is summarised in column 3. In the absence of unconditional data, the distributions for the three key input parameters are defined by **RiskNormal** (mean, stdev, **RiskTruncate** (minimum, maximum)). For example, for the suspended

solids, [conc] =**RiskNormal** (0.115, 0.0023), **RiskTruncate** (0.1104, 0.1196)) which defines a mean value = 0.115 g L<sup>-1</sup>, with stdev = 0.0023 g L<sup>-1</sup> and, respectively, (truncated) minimum and maximum, 0.1104 and 0.1196, g L<sup>-1</sup>.

For each of the key parameters it is seen in Table 5.2 that the truncated minimum and maximum values are defined by  $\pm 2 x$  stdev (stdev = 2 %) about the mean to imitate the most likely practical range of realistic values, and therefore outcomes for *p*. An advantage of using  $\pm 2 x$  stdev on mean value is that 95 % of all sampled values will fall in this interval (Sullivan, 2004; Vose, 2008). Notably, fluctuations in lamp intensity are also simulated with a truncated normal distribution. Lamp intensity will of course not be uniform with time but would be expected to fluctuate with age; it is not clear however whether this aging would in fact be uniform with time (Bolton and Cotton, 2008).

It is seen that the data of column 3 of Table 5.2 are for one-only Fr 13 scenario of the 10,000. All 10,000 are however summarized in Fig. 5.1.

**Table 5.2:** Comparison of traditional SVA with *Fr 13* assessment for UV irradiation inactivation of viable *E. coli* with DL-A kinetics in the presence of UV shielding agent with a % tolerance = 10 % in turbulent flow in the annular reactor.

Parameter	SVA*	Fr 13**	
$I_0 (\mu { m W} { m cm}^{-2})$	55400	54046 <sup>†</sup>	<b>RiskNormal</b> (55400, 1108), <b>RiskTruncate</b> (53184, 57616))
[conc] (g L <sup>-1</sup> )	0.115	$0.115^{\dagger}$	<b>RiskNormal</b> (0.115, 0.0023), <b>RiskTruncate</b> (0.1104, 0.1196))
$Q (\text{mL s}^{-1})$	500	$495.84^{\dagger}$	RiskNormal(500, 10),RiskTruncate(480, 520))
$L(\mathrm{cm})$	196.2	196.2	Constant
$R_1$ (cm)	1.225	1.225	Constant
$R_2$ (cm)	1.74	1.74	Constant
$\mu (\mathrm{kg}\;\mathrm{m}^{-1}\;\mathrm{s}^{-1})$	0.000930	0.000930	Constant
$\rho$ (kg m <sup>-3</sup> )	998.207	998.207	Constant
$v (m^2 s^{-1})$	1.004E-06	1.004E-06	Constant
<i>c</i> (cm)	0.0125	0.0125	Constant
$\alpha$ (cm <sup>-1</sup> )	0.0055	0.0055	Constant

$C_0$	-6.344	-6.344	Constant
$C_1$	-0.0000771	-0.0000771	Constant
$C_2$	7.230E-10	7.230E-10	Constant
$C_3$	-0.685	-0.685	Constant
$v ({\rm cm  s^{-1}})$	104.22	103.35	Eq. (5.6)
$ au_{\mathrm{av}}$ (s)	1.9	1.4	Eq. (5.5)
[dose] (µW s cm <sup>-2</sup> )	104298	102602	Eq. (5.2)
$\ln k (\mu W^{-1}  \mathrm{s}^{-1}  \mathrm{cm}^2)$	-6.5993	-6.5993	Eq. (5.1)
$k (\mu W^{-1}  s^{-1}  cm^2)$	0.001361	0.001361	Eq. (5.1)
$R_{\rm c}$ (dimensionless)	0.8263	0.8263	Eq. (5.7)
d (cm)	0.515	0.515	Eq. (5.8)
Re (dimensionless)	11521	11426	Eq. (5.11)
F (dimensionless)	0.0076	0.0076	Eq. (5.10)
$\delta$ (cm)	243.39	242.89	Eq. (5.9)
$\ln N/N_0$	-2.13	-1.85	Eq. (5.3)
$\log_{10} N/N_0$	-0.92	-0.81	Eq. (5.4)
р		2.829	Eq. (5.12)

\*Traditional single point, or, Single Value, Assessment

\*\* One only of 10,000 scenarios

<sup>†</sup> Values are reproduced from the r-MC sampling; it is not implied they need to be measured to this order

A total 3,205 failures were identified (32.1 %). These can be seen in the right of the figure.

If each simulation is considered one operating day this translates to (3,205/10,000 x)

12 ~) four (4) surprise (unexpected) failures each calendar month, averaged over an

extended period of operation due to the accumulation of combined naturally occurring

random fluctuations in each of [conc],  $I_0$  and Q. It cannot be assumed however these will

actually be spaced evenly in time. Importantly however, this new insight is not provided

by alternative current risk and hazard methodologies, with or without sensitivity analyses.



**Fig. 5.1:** Distribution for the risk factor (*p*) from 10,000 scenarios of UV irradiation for inactivation of viable *E. coli* in the presence of UV shielding agent in turbulent flow in the annular reactor. Failure is defined for all p > 0.

Twenty (20) of these 3,205 failed scenarios are presented in Table 5.3. Row 4 (**bold print**) of the table highlights the particular failed scenario, and combination of parameters, presented in Table 5.2.

**Table 5.3:** Twenty (20) selected failures from 3,205 in 10,000 UV irradiation scenarios forUV shielding agent.

Row	$I_0$ ( $\mu W \text{ cm}^{-2}$ ) <sup>†</sup>	[ <i>conc</i> ] (g L <sup>-1</sup> ) <sup>†</sup>	$Q \ (\mathrm{mL \ s^{-1}})^{\dagger}$	р
1	54493	0.117	497.96	0.066
2	55430	0.112	507.03	0.969
3	54480	0.116	499.05	1.903
<sup>&amp;</sup> 4	54046	0.115	495.84	2.829
5	55048	0.115	505.36	3.703
6	56104	0.116	516.00	4 522
----	-------	-------	--------	--------
6	56184	0.116	516.02	4.533
7	54814	0.112	504.63	5.479
8	53985	0.117	497.57	6.288
9	54835	0.118	505.97	7.426
10	54938	0.116	507.71	8.456
11	54942	0.118	508.44	9.466
12	54076	0.116	501.53	10.544
13	54347	0.113	505.08	11.818
14	53973	0.112	502.79	13.108
15	54655	0.118	509.79	14.492
16	54657	0.117	511.04	15.871
17	54661	0.113	512.71	17.615
18	54428	0.113	512.09	19.289
19	53842	0.115	508.88	21.685
20	53256	0.117	519.74	36.385

<sup>&</sup> particular scenario of Table 5.2
<sup>†</sup> Values are reproduced from the r-MC sampling; it is not implied they need to be measured to this order

#### 5.4. Discussion

### 5.4.1. Model confirmation

Model simulations were extensively tested and were shown to be stable. Given that predicted trends agreed with those published by Abdul-Halim and Davey (2015) over a wide range of inputs it was concluded the simulations were free of programming and computational errors and that the Fr 13 model was therefore suitable for the present purpose.

#### 5.4.2. Ability to identify each Fr 13 event

The advantage of the presentation of the data in Table 5.3 is that the particular combination of UV parameters that resulted in the failure can be readily identified. For example, in row 4 (bold print), the combination of  $I_0 = 54,046 \,\mu\text{W cm}^{-2}$ , [conc] = 0.115 g L<sup>-1</sup> and  $Q = 495.84 \,\text{mL s}^{-1}$  (with corresponding p = 2.829) can easily be read from the table. This ability to easily identify the values of the failure combination means *Fr 13* simulations can be used to quickly screen process effects of key parameters, or impact of proposed interventions and physical changes to the plant.

Importantly, it is not implied that the numerical values reported in Table 5.2 and, especially, Table 5.3, for  $I_0$ , [conc] and Q (with corresponding p) would need to be measured to the stated value (the value is that randomly sampled and used in the r-MC simulations). Further, there is no rationale in the order of presentation of scenarios in Table 5.3, other than the lamp intensity value ( $I_0$ ) is arranged from (row 1) greatest to (row 20) lowest, together with concomitant values of [conc], Q and p. It is not implied that this is the order the events would occur. The use of standard spread sheeting has meant the simulations have been logically ranked by machine from greatest to lowest.

### 5.4.3. Impact of suspended solids

The predicted failure rate in UV efficacy because of the presence of suspended solids as shielding agent (Fig. 5.1) of 32.1 % ( $k = 0.00136 \ \mu W^{-1} \ s^{-1} \ cm^2$ ), averaged over the long term, is less than that for the failure rate for UV absorbing agent ( $k = 0.00146 \ \mu W^{-1} \ s^{-1} \ cm^2$ ) of 43.7 %.

Nevertheless, with both shielding and absorbing solids, the predicted efficacy as  $\log_{10}$  reduction in viable *E. coli* has been reduced to  $\log_{10} \sim 1$  from the  $\log_{10} = 4.35$  without suspended solids present and 16 % failure rate reported by Abdul-Halim and Davey (2015). (This finding resonates with what would be expected).

Significantly, this reduction in viable pathogens falls below the level widely adopted in Regulatory guidelines of a minimum of 4-log<sub>10</sub> (i.e. 99.99 %) (Anon., 2013; Sommer et al., 2008).

An advantage of the *Fr 13* methodology however, is that it can be used in secondtier simulations (Abdul-Halim and Davey, 2015; Davey et al., 2015) to establish quantitatively the impact of changes to the physical system on its vulnerability to failure.

Repeat simulations to quantify the impact of the naturally occurring fluctuations about the mean, and maximum and minimum value, in each of suspended solids concentration as shielding agent, feed water flow, and lamp intensity on UV efficacy in the turbulent flow reactor were therefore carried out for a range  $1 \le \%$ -stdev  $\le 10$ , % in the risk functions (Table 5.2). The risk function used was: **RiskNormal** (mean, stdev), **RiskTruncate** (mean – 2 x stdev, mean + 2 x stdev)) with respective means, [*conc*] = 0.115 g L<sup>-1</sup>, Q = 500 mL s<sup>-1</sup> and  $I_0 = 55,400$  µW cm<sup>-2</sup>. Ten thousand (10,000) simulations were sufficient.

Results are summarized in Fig. 5.2.



**Fig. 5.2:** Impact of %-stdev in distributions for combined, suspended solids as UV shielding agent [*conc*], feed water flow (Q) and lamp intensity ( $I_0$ ), on the number of *Fr 13* failures per 10,000 scenarios in UV irradiation of viable *E. coli* for potable water with DL-A inactivation kinetics in turbulent flow in the annular reactor.

The figure shows that with increasingly tighter control over the variance on the UV reactor parameters, implicit in the figure with deceasing values of %-stdev, the number of predicted *Fr 13* failures decreases nearly exponentially. Tighter and tighter controls will become impractical in the limit however. At values greater than %-stdev ~ 8 % however it is seen that the number of failures begins to plateau to a nearly constant value of 45/10,000 scenarios. However, it is important to note these predictions are for the combined effect of the three key reactor parameters,  $I_0$ , Q and [*conc*], on the UV risk factor, p.

To highlight the individual impact of each, the Spearman rank correlation coefficient (Snedecor and Cochran, 1989), readily available in @*Risk*, can be used, Table 5.4.

**Table 5.4:** Spearman rank correlation coefficient (Snedecor and Cochran, 1989) for the three key input parameters of the annular reactor on UV risk factor (*p*).

<b>Reactor parameter</b>	Coefficient
Q	+0.70
$I_0$	- 0.68
[conc]	+0.03

The data of Table 5.4 show that there is a strong correlation (+ 0.70) between the volumetric flow rate of water (Q, mL s<sup>-1</sup>) and p, and a strong inverse correlation (- 0.68) with lamp intensity ( $I_0$ ,  $\mu$ W cm<sup>-2</sup>).

Conversely and unexpectedly however, it is seen there is a weak correlation (0.03) between suspended solids concentration ([*conc*], g L<sup>-1</sup>) and risk, *p*. That is, although there is an initial highly significant loss of UV efficacy because of suspended solids (respectively, 0.115 and 0.0115, g L<sup>-1</sup> for shielding and absorbing agent) the naturally occurring random fluctuation around this mean concentration in the feed water is not meaningfully impacting UV efficacy and vulnerability to survival of numbers of unwanted viable *E. coli*. The controlling parameter is seen to be the natural fluctuation in feed water flow to the reactor itself (together with fluctuation in lamp intensity).

The effect of UV dose on the reduction of numbers of viable *E. coli*, with DL-A inactivation kinetics (Table 5.1), in the presence of UV shielding agent,  $[conc] = 0.115 \text{ g L}^{-1}$ , in turbulent flow in the annular reactor is summarised in Fig. 5.3 for a range  $80,000 \le [dose] \le 120,000$ ,  $\mu$ W s cm<sup>-2</sup>.

It can be seen from the figure that in the presence of suspended solids as shielding agent a [*dose*] ~ 119,800  $\mu$ W s cm<sup>-2</sup> is necessary to achieve the minimum, Regulatory (Anon., 2013; Sommer et al., 2008) reduction in viable *E. coli* of 4-log<sub>10</sub> (i.e. 99.99 %). For the given UV lamp of intensity  $I_0 = 55,400 \ \mu$ W cm<sup>-2</sup> this translates to a residence time of  $\tau = 2.16$  s necessary for inactivation of viable *E. coli* based on the extensive Amos et al. (2001) data.



**Fig. 5.3:** Impact of UV dose on reduction of numbers of viable *E. coli*, with DL-A inactivation kinetics, in the presence of UV shielding agent,  $[conc] = 0.115 \text{ g L}^{-1}$ , in turbulent flow in the annular reactor.

A direct comparison of these findings with independently reported values e.g. those of Sommer et al. (1998) and Parsons and Jefferson (2009) is problematic simply because these authors do not report the concentration, material (median particle size) or mechanism (as UV shielding/absorbing) of the suspended solids.

#### 5.4.5. Results overview

Practically applied, findings mean that random fluctuations in the feed water flow rate and lamp intensity (possibly increasing with age) have a more significant impact on vulnerability to failure to produce potable water in the annular UV reactor than fluctuations in the suspended solids concentrations as either UV shielding or absorbing, agents.

Ideally however, potable water that is free of suspended solids is a better outcome than extended UV treatment (dose), because these waters will retain (possibly unpleasant tasting and unsightly) suspended solids. Notably, suspended solids of particle sizes greater than about 40 μm will be visible to the naked eye (Allen and Ansel, 2014; Anon., 2007). The UV shielding particles as *Celite 503* of Amos et al. (2001) simulated in this study with a median size 23 μm are about 10 times greater than a typical coliform (Madigan et al., 2003; Anon., 2002) and are not visible to the naked eye. However, in the general case, many suspended solids of this size might impart unwanted taste(s) and odour(s).

A practical response therefore is for a regular and continuous monitoring of suspended solids (possibly using on-line analysers (Pernitsky and Muecci, 2002; Davis and Lettman, 1999)) in the feed water. With refined data and an iterative approach, second-tier simulations could then be readily used to guide engineering decisions on whether the introduction of a pre-filtration step for the feed water to a UV reactor was warranted.

Findings have been interpreted for a daily operation. With batch-continuous processes, say, daily pasteurisation of raw milk with Clean-in-Place (CIP) (Davey et al., 2015), each day can be reasonably thought of as 'one' event, however, UV irradiation for potable water is designed to be largely continuous.

In industrial application, at least two banks of parallel UV reactors would be needed to cover shutdowns and maintenance to give a continuous flow of potable water. A rationale therefore has been to assume a daily basis with a short-time for maintenance – say a possible clean (there are essentially no moving parts) and replacement of the lamp bulb (at say 800 h). Another period however might be used, dependent on what further maintenance is actually required. On a monthly basis for example the reactor(s) might need to be shut down for bulb replacement. However because potable water is a critical utility, it is thought daily calibration checks would actually be needed. (There are strong parallels here with necessary daily operational checks on critical in-line equipment such as industrial gas chromatographs, moisture analysers, etc).

Given that large-scale UV reactors are most likely housed inside a controlled environment (Ultraviolet Technology Australasia Pty Ltd, Australia, *pers. comm.*), it is not considered there will be any significant variations caused to the UV reactor parameters by seasonal change. In any event, the stdev and truncations on the distribution for solids concentration in the feed water [*conc*] = **RiskNormal**(0.115, 0.0023),

**RiskTruncate**(0.1104, 0.1196)) are designed to allow for feed water impacted by seasons. There are no UV parts sensitive to climate conditions (as these are generally quite robust).

Overall, a more unequivocal statement is that 32.1 % of all operations would be expected to fail to produce potable water with the particular UV reactor over the long term.

To confirm the effectiveness of the predictions validation trials against independent literature data, or new data determined experimentally, are needed.

It is nevertheless concluded this work provides strong quantitative evidence for the removal of suspended solids prior to UV inactivation, together with precision control of the feed water flow; rather than an increased UV dose of waters containing suspended solids.

This research with continuous feed water containing suspended solids in a combined pre-treatment filter and UV irradiation reactor is presently under.

### 5.5. Conclusions

The presence of suspended solids, as both UV shielding and UV absorbing agents, has a highly significant initial impact on decreasing the number of viable *E. coli* inactivated in feed water for potable water production in a continuous, turbulent flow 4-series annular UV reactor. The predicted UV efficacy is reduced to approximately one  $\log_{10}$  unit compared to 4.35  $\log_{10}$  units without suspended solids present in the same annular reactor.

The naturally occurring fluctuation in concentration of these solids in combination with lamp intensity ( $I_0$ ) and feed water flow (Q) can result in some 32.1 % and 43.7 % of these continuous UV operations, over the long term, to fail to inactivate a ~ 1-log<sub>10</sub> reduction in numbers of viable *E. coli*.

An unexpected finding, however, is that failure is impacted highly significantly by fluctuation in feed water flow rate and not fluctuations in concentration of solids in the water. It is the initial presence of suspended solids that reduces the practically achievable reduction in coliforms. Practical validation trials against independent literature data or new

data determined experimentally are needed however to confirm the effectiveness of the predictions.

It is concluded that pre-treatment of the feed water to remove (reduce) solids be used to exploit these findings, together with improved control to reduce fluctuation (variance) in the feed water flow to the annular reactor. The generalized model could be used for particular UV irradiation geometries to assess whether a pre-treatment for removal or reduction in solids would be warranted in production of potable water.

The work will be of benefit to operators of UV equipment and researchers in risk analyses.

### Nomenclature

The number in parentheses after description is the equation in which the symbol is defined or first used.

С	correction constant for real reactor, $cm(5.3)$
$C_{\mathrm{i}}$	model coefficients (5.1)
[conc]	suspended solids concentration, g $L^{-1}$ (5.1)
[dose]	UV dose, $\mu$ W s cm <sup>-2</sup> (5.2)
d	annular gap width, cm (5.8)
f	friction factor, dimensionless (5.10)
$I_0$	UV lamp intensity, $\mu$ W cm <sup>-2</sup> (5.2) and (5.3)
k	inactivation constant, $\mu W^{-1} s^{-1} cm^2 (5.1)$
L	length of radiation section, $cm (5.5)$
Ν	concentration viable <i>E. coli</i> , $mL^{-1}$ (5.3) and (5.4)
$N_0$	concentration viable <i>E. coli</i> before UV exposure, $mL^{-1}$ (5.3) and (5.4)
р	UV risk factor, dimensionless (5.12)
Q	volumetric flow rate, mL s <sup><math>-1</math></sup> (5.6)
$R_1$	radius of inner cylinder, cm $(5.6)$ , $(5.7)$ and $(5.8)$
$R_2$	radius of outer cylinder, cm $(5.6)$ , $(5.7)$ and $(5.8)$
R <sub>c</sub>	dimensionless group (5.7)
Re	Reynolds number, dimensionless (5.11)
V	average water velocity in annular gap, cm s <sup>-1</sup> $(5.6)$
Greek	
α	absorption coefficient, $cm^{-1}$ (5.3)
δ	boundary layer thickness, cm $(5.3, 5.9)$

$\mu$ uynamic viscosity of water, 0.75 x 10 Kg m s (J.	μ	dynamic viscosity of water, 0.93 x $10^{-3}$ kg m <sup>-1</sup> s <sup>-1</sup>	(5.9
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- $\rho$  density of water at 20 °C, 998.207 kg m<sup>-3</sup> (5.9)
- $\tau$  residence (exposure) time, s (5.2, 5.5)
- v kinematic viscosity of water at 20 °C, 1.004 x 10<sup>-6</sup> m<sup>2</sup> s<sup>-1</sup> (5.9)

Other

%tolerance practical tolerance (margin) in reduction in viable E. coli, % (5.12)

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# A GLOBAL MICROBIAL RISK MODEL FOR ESCHERICHIA COLI IN TWO-STEP SAND-FILTRATION AND ULTRAVIOLET IRRADIATION (SF-UV) FOR POTABLE WATER IN AN ANNULAR REACTOR

## A GLOBAL MICROBIAL RISK MODEL FOR *ESCHERICHIA COLI* IN TWO-STEP SAND-FILTRATION AND ULTRAVIOLET IRRADIATION (SF-UV) FOR POTABLE WATER IN AN ANNULAR REACTOR

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- i. the candidate's stated contribution to the publication is accurate (as detailed above);
- ii. permission is granted for the candidate in include the publication in the thesis; and
- iii. the sum of all co-author contributions is equal to 100 % less the candidate's stated contribution

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### Abstract

Ultraviolet (UV) irradiation is an important alternative to chemical disinfection for potable water production. However it is known that suspended solids (SS) concentration in the raw feed-water can reduce standalone UV reactor efficacy (Chem. Eng. Sci. 143 (2016) 55-62), and therefore integrated pre-treatment of SS with rapid sand-filters (SF) is sometimes used. Here we synthesize a Fr 13 risk assessment for a two-step integrated SF-UV for the first time. The aim was to investigate how naturally occurring, random (stochastic) fluctuations in apparent steady-state plant parameters could be transmitted and impact UV efficacy in an annular reactor for production of potable water. The approach was to define SF-UV behavior through a unit-operations model and simulate this using a refined Monte Carlo (with Latin Hypercube) sampling of SS and feed-water flow rate (Q). Overall failure of the integrated two-step SF-UV is defined as unwanted levels of survival of viable E. coli, a widely used indicator for public health risk. Results show the overall vulnerability to failure of SF-UV operations is 40.4 %. This equates to 148 failures per annum averaged over the long term, if each scenario is considered a daily operation. These failures are not expected to be spaced equally in time however. The mean reduction of SS in SF was  $log_{10}$ -1.11 (90 %), with a subsequent reduction of viable E. coli in the UV reactor of  $log_{10}$ -2.93 (99.9 %). This is a highly significant increase in UV efficacy compared with that ( $\log_{10}$  -0.92) without pre-treatment of the raw feed-water. SF-UV is shown to be a mix of successful and failed operations, and; significantly that not all failed SF automatically result in failure in overall UV process efficacy. This new insight is not available from alternate risk assessments. Second-tier simulation showed that the higher the safety tolerance the greater the loss of flexibility in SF-UV reactor. Precision control is therefore suggested to minimize vulnerability of these unexpected failures. The work will be of

149

immediate interest to risk analysts, and benefit to operators and managers responsible for the production of potable water using UV irradiation.

### Keywords:

ultraviolet irradiation for potable water; rapid sand filtration; failure of UV irradiation; risk assessment; Friday 13<sup>th</sup> risk modelling; *Fr 13* risk

### HIGHLIGHTS

- *Fr 13* risk framework applicable to integrated SF-UV for potable water production.
- Stochastic effects cause of unwanted levels of survival of *E. coli*.
- SF-UV shown to be mix of successful and failed operations.
- Integrated SF-UV highly significantly improves UV efficacy over UV standalone.
- Immediate benefit to risk analysts, water processors and designers of UV reactors.

### 6.1. Introduction

Ultraviolet (UV) irradiation is becoming an important alternative to chemical disinfection for potable water production (Abdul-Halim and Davey, 2016; Das, 2001). Steady-state operation is widely used in which the process risk to public health is, almost universally, defined as a failure to reduce the levels of viable *Escherichia coli*, a fecal and pathogenic bacterium, in the raw feed-water (Amos et al. 2001).

However in apparent steady-state operations there will be naturally occurring random (stochastic) fluctuations in plant parameters about the 'set' steady-value. In traditional chemical engineering these fluctuations are not considered as transient, or significant, but rather, problematic. Generally, it is widely thought that these will be compensated for by corresponding fluctuations in other parameters - with the result that the overall plant output behavior will be seemingly unchanged (Zou and Davey, 2016).

Importantly however Davey and co-workers have shown that plant failure can unexpectedly result from an accumulation of these naturally occurring fluctuations in one direction (e.g. Davey et al., 2013; Chandrakash et al., 2015; Davey et al., 2015; Davey, 2011). They coined the descriptor *Friday*  $13^{th}$  syndrome (*Fr* 13) to underscore the surprise and unexpected nature of these events. Major advantages claimed for the *Fr* 13 risk framework include that it 1) provides unique and quantitative insight into the underlying plant outcomes behavior, and; 2) can be used to devise process intervention strategies and careful re-design of physical plant to reduce risk through 'second-tier' studies (Zou and Davey, 2016). This is because the framework is predicated on widely established unitoperations processing (Foust et al., 1980; Ozilgen, 1998; McCabe et al., 2001). Moreover, it can be applied in both the *analysis* and *synthesis* stages (Turton et al., 2009). According to the Blackett Review (Anon., 2012), these low-probability, high-impact failures are an emerging challenge for processors and governments - especially because of ever increasing inter-connectedness of product and downstream processing world-wide.

In applying the *Fr 13* framework to UV irradiation for potable water production Abdul Halim and Davey (2015) demonstrated that over the long-term some 16 % of all continuous steady-state UV plant operations in an annular reactor with turbulent flow (Re > 4,000) will fail to achieve a design reduction of  $\log_{10}$  -4.35 in contaminant viable *E. coli* as a result of the accumulated impact of random effects in feed-water flow rate (*Q*), UV lamp fluence (*I*<sub>0</sub>) and inactivation rate (*k*) for the viable pathogen. Their analysis was based on the extensive independent data of Ye (2007) - and was shown to be an advance on current risk assessments because it produced all practical UV plant behaviour outcomes, including failure of UV efficacy.

It has long been known however that contaminant pathogens can be protected, either through shielding from UV by suspended solids (SS) in the feed-water, or, through UV absorbing on these solids. The practical upshot is that that UV efficacy is increasingly reduced with increasing concentrations of SS (Qualls et al., 1983; Amos et al., 2001).

Abdul Halim and Davey (2016), in a detailed study, applied the *Fr* 13 risk framework to UV irradiation of feed-water containing a range of concentration of both UV shielding and UV absorbing suspended solids (respectively, 0.115 and 0.0115, g L<sup>-1</sup> with median particle size 23 µm) that was irradiated in an annular reactor with turbulent feedwater flow (Re > 11,000). They defined a UV failure factor in terms of the design, and actual, log<sub>10</sub> reduction in viable *E. coli*. Based on the experimental data of Amos et al. (2001) for *E. coli* (ATCC 25922 'Seattle' strain) they showed that the accumulated impact of naturally occurring fluctuations in concentration ([*conc*]) of SS, feed-water flow rate (*Q*) and UV lamp fluence (*I*<sub>0</sub>) could be, respectively, some 32.1 and 43.7, % of apparent successful operations would unexpectedly fail. This translated to about four (4) failures each calendar month, averaged over the long term. An unexpected finding was that although the initial presence of SS as both UV shielding and UV absorbing agent had a highly significant impact on reducing process efficacy (from log<sub>10</sub> 4.35 to 0.99), fluctuations in concentration of these SS did not meaningfully impact overall vulnerability to failure of UV reactor operation. They concluded that the findings were strong quantitative evidence that solids should be removed from the feed-water prior to the UV reactor, and; that there was a need for high-level flow control on the feed-water rather than an increase in applied UV dose.

In conventional processing pre-treatment with rapid sand-filtration (SF) is sometimes used to remove SS prior to sequential UV irradiation (Liltved and Cripps, 1999; Abdul-Halim and Davey, 2016). This involves passing a steady-flow of raw feed-water through a granular bed of sand. The sand retains the physical contaminants whilst allowing treated water to pass through. Particles that are removed are typically in the < 50  $\mu$ m range; these are much smaller than that of the sand-filter media of 500 to 2,000,  $\mu$ m (Parsons and Jefferson, 2009). With this steady-state, two-step SF-UV sequential treatment the overall treatment efficacy for potable water is enhanced with reduced risk of unwanted survival of water-borne microbial pathogens i.e. a decreased failure risk of UV irradiation for potable water production.

It is not known however what impact pre-treatment of the feed-water with a rapid SF will have on the overall risk to the efficacy of a sequential (integrated) SF-UV reactor.

### 6.1.1. Purpose of this study

Here we extend for the first time the Fr 13 risk framework to investigate the impact on overall efficacy of a sequential SF-UV process for production of potable water. A global two-step model is synthesized for the integrated SF-UV. We solve this extended synthesis to quantify a realistic failure probability for unwanted survival of a viable contaminant pathogen. We illustrate the global model with independent, published data for *E. coli* (ATCC 25922) and demonstrate it in second-tier studies (Abdul Halim and Davey, 2016) to re-assess design to limit vulnerability to surprise failure and unwanted survival of viable *E. coli*.

This research will be of immediate interest to risk analysts, and benefit to operators and managers responsible for the production of potable water using UV irradiation. It was hoped findings could be generalized to a range of reactor geometries.

### 6.2. Materials and methods

A conventional unit-operations model for water treatment is shown schematically in Fig. 6.1. The integrated and sequential SF-UV unit-operations can be readily seen from the figure.

An adequate model for the SF-UV requires integration of equations for the removal of solids in the filter, together with those for UV inactivation of the contaminating *E. coli* and hydrodynamic flow in the annular UV reactor. In the following, these are treated separately then synthesized into the global two-step model for integrated SF-UV for production of potable water. All symbols used are carefully defined in the Nomenclature.



**Fig. 6.1:** Schematic of conventional treatment for potable water production. Highlighted is the integrated SF-UV unit-operations.

### 6.2.1. Rapid sand-filter (SF)

Rapid sand-filtration of SS is dependent on a number of properties, including the: filter bed (grain shape and size distribution, porosity, depth); influent suspension (turbidity, concentration; particle size distribution; particle and water density; water viscosity; temperature and level of pre-treatment), and; operating conditions (filtration rate) (Howe et al., 2012). Particles are removed throughout the filter by transport mechanisms and attachment (Crittenden et al., 2012; Howe et al., 2012).

A schematic for rapid sand-filtration for particle removal is presented as Fig. 6.2.

The SS concentration in the feed-water influent,  $[conc]_{SF0}$ , is seen to pass through the filter-bed of cross-sectional area, A, and depth,  $L_{SF}$ , at a volumetric flow rate, Q, to give a resulting effluent SS concentration,  $[conc]_{SF}$ .



Fig. 6.2: Rapid sand-filtration (SF) for SS removal.

Crittenden et al. (2012) developed an advanced filtration model based on the work by Yao et al. (1971) for SS removal that is given by

$$[conc]_{SF} = [conc]_{SF0} \exp\left[\frac{-3(1-\varepsilon)\alpha_{\rm E}\eta L_{SF}}{2dc}\right]$$
(6.1)

in which the total transport efficiency,  $\eta$ , is given by

$$\eta = \eta_{\rm I} + \eta_{\rm G} + \eta_{\rm D} \tag{6.2}$$

and where the transport efficiency due to interception,  $\eta_{I}$ , is

$$\eta_I = \frac{3}{2} N_R^2 \tag{6.3}$$

156

in which the relative size group,  $N_{\rm R}$ , is

$$N_{\rm R} = \frac{dp}{dc} \tag{6.4}$$

Transport efficiency due to gravity,  $\eta_{\rm G}$ , is given as

$$\eta_{\rm G} = N_{\rm G} \tag{6.5}$$

where the gravity number,  $N_{\rm G}$ , is

$$N_{\rm G} = \frac{V_{\rm S}}{V_{\rm G}} = \frac{g(\rho_p - \rho_w)dp^2}{18\mu V_{\rm F}}$$
(6.6)

The filtration rate,  $V_{\rm F}$ , is defined as

$$V_{\rm F} = \frac{Q}{A} \tag{6.7}$$

where Q is the volumetric flow rate, and; A is the cross-sectional area of the filter given by

$$A = L_{\rm SF} \times W \tag{6.8}$$

The transport efficiency due to diffusion,  $\eta_D$ , is given by

$$\eta_{\rm D} = 4Pe^{-2/3} \tag{6.9}$$

in which the Peclet number is defined as

$$Pe = \frac{3\pi\mu dp V_{\rm F}}{K_B T} \tag{6.10}$$

Substituting Eq. (6.10) into Eq. (6.9) gives

$$\eta_D = 4 \left(\frac{3\pi\mu dp V_F}{K_B T}\right)^{-2/3} \tag{6.11}$$

157

The  $log_{10}$  reduction in SS concentration is given by

$$\log \frac{[conc]_{SF}}{[conc]_{SF0}} = \frac{\ln \frac{[conc]_{SF}}{[conc]_{SF0}}}{2.303}$$
(6.12)

#### 6.2.2. UV inactivation of viable E. coli

Extensive experimental data (n = 40) and analyses for UV inactivation of *E. coli* (ATCC 25922, Seattle) in the presence of SS was presented by Amos et al. (2001). A commercial UV Unit (Model LC-5, Ultraviolet Technology Australasia Pty Ltd, Australia) was used. The SS were diatomaceous earth (as *Celite* 503<sup>TM</sup>) for controlled UV shielding (89 % SiO<sub>2</sub> with median particle size 23  $\mu$ m), and coffee powder (International Roast<sup>TM</sup>) for controlled UV absorbing.

Four (4) model forms were evaluated including the, Classical log-linear, Davey linear-Arrhenius (DL-A) (Ross and Dalgaard, 2004; McMeekin et al., 1993; Davey, 1993), Square-root (i.e. Ratkowsky-Belehradek) (Ratkowsky, 1990; Belehradek, 1926), and; a third-order Polynomial (*n*OP). Models were ranked on the goodness of fit (percent variance accounted for (%V) (Snedecor and Cochran, 1989), relative complexity (i.e. parsimony) (McMeekin et al., 1993; Davey, 1993), ease of synthesis and use, and; potential for physiological interpretation of coefficients.

The DL-A was shown to best fulfill the test criteria (%V = 97.2) and a predictive model for inactivation with both UV shielding and UV absorbing solids was synthesized of the following form

$$\ln k = C_0 + C_1 [dose] + C_2 [dose]^2 + C_3 [conc]_{SF-UV}$$
(6.13)

where  $[conc]_{SF} = [conc]_{SF-UV}$ , and in which UV dose [dose] is given by

$$[dose] = I_0 \tau \tag{6.14}$$

The applicable range for this model for shielding agent is  $0.01 \le [conc]_{SF-UV} \le 0.3$ , g L<sup>-1</sup>.

The model form is said to be linear-Arrhenius and 'additive' (Ross and Dalgaard,

2004; Davey, 1993; Amos et al., 2001). The values for the model coefficients  $(C_0 - C_3)$  for UV inactivation of viable *E. coli* in the presence of UV shielding are given in Table 6.1.

**Table 6.1:** Coefficients for the Davey linear-Arrhenius (DL-A) model for UV irradiation inactivation of viable *E. coli* (ATCC 25922 'Seattle' strain) in the presence of suspended solids as UV shielding agent (Amos et al., 2001) in which

$$\ln k = C_0 + C_1[dose] + C_2[dose]^2 + C_3[conc]_{SF-UV}$$

with k in  $\mu$ W<sup>-1</sup> s<sup>-1</sup> cm<sup>2</sup> for a range of concentration of shielding agent 0.01  $\leq$  [conc]  $\leq$  0.3, g L<sup>-1</sup>

C <sub>0</sub>	$C_1 \ge 10^{-4}$	$C_2 \ge 10^{.9}$	<i>C</i> <sub>3</sub>
- 6.344	- 0.771	0.723	- 0.685

### 6.2.3. Concentric annular UV reactor

A steady-state plug-flow (PFR) concentric annular-reactor for UV irradiation of turbulent flow of water was presented by Abdul-Halim and Davey (2015; 2016) based on the work of Ye (2007) such that the reduction in contaminant viable *E. coli* was given by

$$\ln\left(\frac{N}{N_0}\right) = -\frac{ckI_0\tau R_c}{\alpha d\delta} \tag{6.15}$$

For a more convenient  $log_{10}$  base, Eq. (6.15) was written as

$$\log_{10}\left(\frac{N}{N_0}\right) = \frac{\ln\left(\frac{N}{N_0}\right)}{2.303}$$
(6.16)

The residence time of the water in the reactor was given by

$$\tau = \frac{L}{v} \tag{6.17}$$

with water velocity in concentric annular gap defined by

$$\nu = \frac{Q}{\pi (R_2^2 - R_1^2)} \tag{6.18}$$

A dimensionless group for the inner cylinder was defined by Ye (2007) as

$$R_c = \frac{2R_1}{R_1 + R_2} \tag{6.19}$$

The annular gap dimension is defined by

$$d = R_2 - R_1 \tag{6.20}$$

The ratio  $(c/\delta)$  (Eq. (6.15)) was used by Ye (2007) to correct for deviation of the real reactor from a PFR. From the data of Ye (2007) c = 0.0125 cm.

The boundary layer for turbulent flow  $(\delta)$  is

$$\delta = \frac{2\mu}{\rho_w v f} \tag{6.21}$$

The friction factor (*f*) is given by

$$f = 0.079 \,\mathrm{Re}^{-0.25} \tag{6.22}$$
where

$$\text{Re} = 2d\rho v/\mu \ge 2,100$$
 (6.23)

in which 2*d* is the hydraulic diameter for the concentric annulus (outer – inner, cylinder diameter). The transition from laminar to turbulent flow occurs when  $2,100 \le \text{Re} \le 4,000$  and a fully developed turbulent flow when  $\text{Re} \ge 4,000$  (Koutchma et al., 2009).

#### 6.2.4. SF-UV global model

Eqs. (6.1) through (6.23) define the integrated (global) SF-UV steady-state operation for continuous production of potable water with feed-water flow with suspended solids together with contaminating viable *E. coli* in turbulent flow in the annular UV reactor.

#### 6.3. Traditional, deterministic Single Value Assessment (SVA)

The traditional solution approach is the deterministic, single point or Single Value Assessment (SVA), with or without sensitivity analyses (Sinnott, 2005). For a given raw feed-water SVA computations for the integrated SF-UV proceed as follows:

For removal of SS in SF; the initial concentration of SS in feed flow is  $[conc]_{SF0} = 0.115 \text{ g L}^{-1}$  (Amos et al., 2001). From the data of Crittenden et al. (2012);  $L_{SF} = 40 \text{ cm}$ , W = 200 cm,  $\varepsilon = 0.380$  (dimensionless),  $\alpha_{E} = 0.5$  (dimensionless), dc = 0.02 cm, and  $dp = 2.3 \text{ x } 10^{-5} \text{ cm}$ , Substituting into Eq. (6.4) gives  $N_{R} = 1.15 \text{ x } 10^{-3}$  (dimensionless) and  $\eta_{I} = 1.984 \text{ x } 10^{-6}$  (dimensionless), from Eq. (6.3). Given,  $Q = 450 \text{ cm}^{3} \text{ s}^{-1}$ , yields  $A = 8,000 \text{ cm}^{2}$  and  $V_{F} = 0.00563 \text{ cm s}^{-1}$  from Eq. (6.8) and Eq. (6.7), respectively. Using  $g = 981 \text{ cm s}^{-2}$ , and

for water at 20 °C,  $\rho_p = 1.442 \text{ x } 10^{-3} \text{ kg cm}^{-3}$ ,  $\rho_w = 9.98 \text{ x } 10^{-4} \text{ kg cm}^{-3}$ ,  $\mu = 9.3 \text{ x } 10^{-6} \text{ kg}$ cm<sup>-1</sup> s<sup>-1</sup> (Kestin et al., 1978), yields  $\eta_G = N_G = 2.446 \text{ x } 10^{-5}$  (dimensionless) from Eq. (6.5) and (6.6). Given  $K_B = 1.381 \text{ x } 10^{-19} \text{ kg cm}^2 \text{ s}^{-2} \text{ K}^{-1}$  and T = 293 K, yields Pe = 5.606 x  $10^4$ (dimensionless) from Eq. (6.10) and; from Eq. (6.11)  $\eta_D = 2.731 \text{ x } 10^{-3}$  (dimensionless). The total transport efficiency,  $\eta = 2.757 \text{ x } 10^{-3}$  (dimensionless) is obtained from Eq. (6.2). The concentration of effluent with SS is computed from substituting the values for [*conc*]<sub>SF0</sub>,  $\varepsilon$ ,  $\eta$ ,  $\alpha_E$ ,  $L_{SF}$ , and *dc* to yield [*conc*]<sub>SF</sub> = 0.00885 g L<sup>-1</sup> in Eq. (6.1). The log reduction in SF is computed from Eq. (6.12) to give  $\log_{10} = -1.11$  - which is > 90 % of reduction in viable *E. coli*.

Similarly, the SVA or the turbulent flow annular UV reactor defined by  $I_0 = 55,400$   $\mu$ W cm<sup>-2</sup>, Q = 450 cm<sup>3</sup> s<sup>-1</sup>, L = 196.2 cm,  $R_1 = 1.225$  cm and  $R_2 = 1.74$  cm, and for the inactivation of viable *E. coli* defined by the model coefficients for UV shielding (Amos et al., 2001) where  $C_0 = -6.344$ ,  $C_1 = -0.771 \times 10^{-4}$ ,  $C_2 = 0.723 \times 10^{-9}$ , and  $C_3 = -0.685$  (Table 6.1). From Eq. (6.18) v = 93.79 cm s<sup>-1</sup>;  $\tau = 2.1$  s from Eq. (6.17), and; [*dose*] = 115,887  $\mu$ W s cm<sup>-2</sup> from Eq. (6.14). Substitution for [*conc*]<sub>SF</sub> = [*conc*]<sub>SF-UV</sub> = 0.00885 g L<sup>-1</sup>, k =0.00379  $\mu$ W<sup>-1</sup> s<sup>-1</sup> cm<sup>2</sup> from Eq. (6.13). Calculations for Eq. (6.19) and Eq. (6.20) respectively yields  $R_c = 0.8263$  (dimensionless) and d = 0.515 cm. Substitute  $\mu = 9.3 \times 10^{-6}$ kg cm<sup>-1</sup> s<sup>-1</sup> and  $\rho_w = 9.98 \times 10^{-4}$  kg cm<sup>-3</sup> gives Re = 10,369 (dimensionless) from Eq. (6.23) and from Eq. (6.22) f = 0.0078 (dimensionless). The value of the kinematic viscosity of water (20 °C) used is v = 0.01 cm<sup>2</sup> s<sup>-1</sup> (Crittenden et al., 2012). Substitution together with the value for *f* into Eq. (6.21) gives  $\delta = 237.07$  cm. The reduction in the number of viable *E. coli* is computed from substitution of values for [*conc*]<sub>SF-UV</sub>, k,  $I_0$ ,  $\tau$ ,  $R_c$ , a, d and  $\delta$  into Eq. (6.15) to give ln  $N/N_0 = -6.76$  (dimensionless). From Eq. (6.16) therefore  $\log_{10} N/N_0 = -$ 2.93 (dimensionless) (99.9 %). A summary of the SVA for each of SF and UV is presented in Table 6.2. The

**bolded text** (column 2, row 26 and column 5, row 17) is used to highlight that the output concentration from SF is actually the input concentration to the sequential and integrated UV reactor.

**Table 6.2:** Traditional single value assessment (SVA) for global SF-UV inactivation of *E*.

 *coli* in feed-water flow.

	Unit-operation						
San	nd-filter (SF)		UV reactor (UV)				
Parameter			Parameter				
$L_{\rm SF}$ (cm)	40	constant	L(cm)	196.2	constant		
W(cm)	200	constant	$R_1$ (cm)	1.225	constant		
$\varepsilon$ (dimensionless)	0.380	constant	$R_2$ (cm)	1.74	constant		
$\alpha_{\rm E}$ (dimensionless)	0.50	constant	$\mu$ (kg cm <sup>-1</sup> s <sup>-1</sup> )	9.3E-06	constant		
dc(cm)	0.02	constant	$\rho_{\rm w}$ (kg cm <sup>-3</sup> )	9.98E-04	constant		
dp (cm)	2.3E-05	constant	$v (\rm{cm}^2 \rm{s}^{-1})$	0.01	constant		
$\rho_{\rm p} ({\rm kg}{\rm cm}^{-3})$	1.442E-03	constant	<i>c</i> (cm)	0.0125	constant		
$\rho_{\rm w}$ (kg cm <sup>-3</sup> )	9.98E-04	constant	$\alpha$ (cm <sup>-1</sup> )	0.0055	constant		
$\mu$ (kg cm <sup>-1</sup> s <sup>-1</sup> )	9.3E-06	constant					
$g ({\rm cm  s^{-2}})$	981	constant	<u>E. coli</u>				
$K_{\rm B}$ (kg cm <sup>2</sup> s <sup>-2</sup> K <sup>-1</sup> )	1.381E-19	constant	$C_0$	-6.344	constant		
$T(\mathbf{K})$	293	constant	$C_1$	-0.0000771	constant		
- ()			$C_2$	7.230E-10	constant		
			$C_3$	-0.685	constant		
			- 5				
$[conc]_{SF0}$ (g L <sup>-1</sup> )	0.115	input	$I_0 (\mu W  \mathrm{cm}^{-2})$	55400	input		
$Q (\text{cm}^3 \text{ s}^{-1})$	450	input	$[conc]_{SF-UV}$ (g L <sup>-1</sup> )	0.0885	input		
~ ` `		1	$Q(\text{cm}^3 \text{s}^{-1})$	450	input		
					-		
Computations			Computations				
$N_{\rm p}$ (dimensionless)	1 150E-03	$F_{0}(64)$	$v (cm s^{-1})$	93 79	$E_{0}$ (6.18)		
$n_{\rm I}$ (dimensionless)	1.984E-06	Eq. $(6.3)$	$\tau$ (s)	2.1	Eq. $(6.17)$		
$A (cm^2)$	8000	Eq. $(6.8)$	[dose] (uW s cm <sup>-2</sup> )	115887	Eq. $(6.14)$		
$V_{\rm F} ({\rm cm}{\rm s}^{-1})$	0.0563	Eq. $(6.7)$	$\ln k (uW^{-1} s^{-1} cm^2)$	-5.575	Eq. $(6.13)$		
$n_{\rm C}$ (dimensionless)	2.446E-05	Eq. (6.6)	$k (uW^{-1} s^{-1} cm^2)$	0.00379	Eq. (6.13)		
Pe (dimensionless)	5.606E+04	Eq. (6.10)	$k (\text{mW}^{-1} \text{ s}^{-1} \text{ cm}^2)$	3.791	Eq. (6.13)		
$\eta_{\rm D}$ (dimensionless)	2.731E-03	Eq. (6.11)	$R_{\rm c}$ (dimensionless)	0.8263	Eq. (6.19)		
$\eta$ (dimensionless)	2.757E-03	Eq. (6.2)	d (cm)	0.515	Eq. (6.20)		
- · · /		<u> </u>	Re (dimensionless)	10369	Eq. (6.23)		
			f(dimensionless)	0.0078	Eq. (6.22)		
[conc] <sub>SF</sub>	0.0885	Eq. (6.1)	$\delta$ (cm)	237.07	Eq. (6.21)		
					·		
			$\ln N/N_0$	-6.757	Eq. (6.15)		
			$\log_{10} N/N_0$	-2.93	Eq. (6.16)		

#### 6.4. Fr 13 model simulations

#### 6.4.1. Failure factors

A requirement in the *Fr* 13 risk assessment framework is an unambiguous definition of failure (Chandrakash et al., 2015). For the rapid SF, a risk factor for vulnerability to failure to reduce SS can be mathematically defined in terms of  $[conc]_{SF}$ ' and  $[conc]_{SF}$  such that  $p = [conc]_{SF}' - [conc]_{SF}$ .

This can be rearranged (Zou and Davey, 2016) to a dimensionless and more convenient form as

$$p_1 = 100 \left( 1 - \frac{[conc]_{\rm SF}'}{[conc]_{\rm SF}} \right) \tag{24a}$$

where  $[conc]_{SF}$ ' is an instantaneous value of  $[conc]_{SF}$  (or more mathematically correct, one possible scenario). However operations would, generally, include a production tolerance (margin of safety) such that  $[conc]_{SF}$ ' needs to be equal to the minimum required value, plus an additional *tolerance* such that

$$p_1 = -\% tolerance + 100 \left(1 - \frac{[conc]_{\rm SF}'}{[conc]_{\rm SF}}\right)$$
(24)

A risk factor for failure of UV was defined by Abdul-Halim and Davey (2015, 2016) and is given by

$$p_{2} = -\% tolerance + 100 \left[ 1 - \frac{\log_{10} \left( \frac{\dot{N}}{N_{0}} \right)}{\log_{10} \left( \frac{N}{N_{0}} \right)} \right]$$
(25)

where  $\log_{10}\left(\frac{\dot{N}}{N_0}\right)$  is an instantaneous value of  $\log_{10}\left(\frac{N}{N_0}\right)$ . A practical process tolerance of 10 % on the required  $\log_{10}$  reduction of viable *E. coli* is assumed (Abdul-Halim and Davey, 2015, 2016) i.e. if the design  $\log_{10}$  reduction in viable *E. coli* plus 10 % is not achieved, the UV treatment is said to have failed. The tolerance is therefore a margin of safety.

It can be seen that Eqs. (24) and (25) are computationally convenient because, respectively, for all  $p_1 > 0$  treatment for removal of the required level of SS will have failed, and, for all  $p_2 > 0$ , UV treatment for potable water production will have failed.

#### 6.4.2. Fr 13 simulations

In *Fr 13* simulations the single value for model parameters is replaced by a probability distribution of values, the mean of which generally agrees with the SVA (Zou and Davey, 2016; Abdul-Halim and Davey, 2015, 2016). A refined Monte Carlo (with Latin Hypercube) sampling is used (r-MC). r-MC is used because 'pure' Monte Carlo can overestimate and underestimate samples from a parts of the distribution (*see* Zou and Davey (2016) & Abdul-Halim and Davey (2015) for a brief discussion). If the number of samples is sufficiently large the output will be approximately normally distributed (Vose, 2008). To ensure that the output distribution is normal, a minimum number of samples are necessary, usually, this is some 1,000 to 50,000 samples (Abdul-Halim and Davey, 2016; Zou and Davey, 2016).

Importantly, because a large number of samples are used, it can be reasonably concluded that all process scenarios that can actually occur in practical plant operation, including, any plant failures, will be included.

Generally there are some 40 types of probability distribution exist (Zou and Davey, 2016). In absence of expert knowledge Truncated-Normal is used - previous

experimentation with different distributions (e.g. Pert) showed no meaningful change to failure rate (Davey, 2015; Abdul-Halim and Davey, 2016). The value of key parameters, concentration of SS ([*conc*]) and raw feed-water flow (*Q*) are assumed normally distributed in the absence of unconditional data. The distribution is defined as **RiskNormal** [mean, standard deviation, **RiskTruncate** (minimum, maximum)]. Truncation is used to set practical limits on values that might actually occur in actual process operations.

The calculations were performed in Microsoft Excel<sup>TM</sup> and *Fr 13* simulations carried out with commercially available add-on @*Risk* (version 5.5, Palisade Corporation<sup>TM</sup>).

A benefit of using spread sheeting is the process of communicating results is streamlined because these are used almost universally. Additionally, the distributions can be entered, copied, pasted and viewed as Excel formulae.

#### 6.5. Results

A comparative summary of the results from both the traditional deterministic SVA and probabilistic Fr 13 simulation for the rapid sand-filtration are presented in Table 6.3. Ten thousand (10,000) random samples from the distributions were found sufficient. Each simulation can be considered a daily SF process to remove SS in the feed-water. Key parameters are given in column 1 of the table.

Table 6.3: Comparison of traditional SVA with Fr 13 risk assessment for particle removal

Parameter	<b>SVA</b> <sup>a</sup>		Fr 13 <sup>b</sup>
$[\operatorname{conc}]_{\operatorname{SF0}}(\operatorname{gL}^{-1})$	0.115	0.100	RiskNormal(0.115,0.0069),RiskTruncate(0.0943,0.1357)
Q (cm <sup>3</sup> s <sup>-1</sup> )	450	456	RiskNormal(450,27),RiskTruncate(369,531)
L <sub>SF</sub> (cm)	40.00	40.00	constant
W (cm)	200.00	200.00	constant
$\epsilon$ (dimensionless)	0.380	0.380	constant
$\alpha_{\rm E}$ (dimensionless)	0.50	0.50	constant
$d_{\rm C}({\rm cm})$	2.000E-02	2.000E-	constant
$d_{\rm P}({\rm cm})$	2.300E-05	2.300E-	constant
$\rho_{\rm P}$ (kg cm <sup>-3</sup> )	1.442E-03	1.442E-	constant
$\rho_{\rm W}$ (kg cm <sup>-3</sup> )	9.98E0-4	9.98E0-4	constant
$\mu$ (kg cm <sup>-1</sup> s <sup>-1</sup> )	9.30E-06	9.30E-06	constant
$g (cm s^{-2})$	981	981	constant
$K_{\rm B} ({\rm kg} {\rm cm}^2 {\rm s}^{-2} {\rm K}^{-1})$	1.381E-19	1.381E-	constant
T (K)	293	293	constant
Computations			
N <sub>R</sub> (dimensionless)	1.150E-03	1.150E-	Eq. (6.4)
$\eta_{\rm I}$ (dimensionless)	1.984E-06	1.984E-	Eq. (6.3)
$A(cm^2)$	8000	8000	Eq. (6.8)
$V_{\rm F} ({\rm cm \ s}^{-1})$	0.0563	0.0570	Eq. (6.7)
$\eta_G$ (dimensionless)	2.446E-05	2.414E-	Eq. (6.6)
Pe (dimensionless)	5.606E+04	5.683E+0	Eq. (6.10)
$\eta_D$ (dimensionless)	2.731E-03	2.706E-	Eq. (6.11)
$\eta$ (dimensionless)	2.757E-03	2.732E-	Eq. (6.2)
$\left[ \operatorname{concl} \left( \operatorname{g} \mathbf{I}^{-1} \right) \right]$	0.00805	0.00789	$\mathbf{F}_{\mathbf{G}}$ (6.1)
p	0.00883	0.00788 1 00°	Eq. $(0.1)$
$P_1$		1.00	Eq. (0.24)

in rapid sand-filtration (SF) with a % tolerance (safety margin) = 10 %.

Deterministic Single Value Assessment. b

Fr 13 simulation with Latin Hypercube sampling.

Values are reproduced as exactly those from r-MC sampling; it is not implied they need to be measured in this order.

The traditional SVA is read down column 2 where the output SS concentration for rapid SF,  $[conc]_{SF} = 0.00885 \text{ g L}^{-1}$  is shown. Columns 3 and 4 are the *Fr 13* simulation. The distributions for input parameters ( $[conc]_{SF0}$  and Q) are presented in column 4. It can be seen from the table that for the input SS concentration in rapid SF,  $[conc]_{SF0} = 0.115$  g  $L^{-1}$  and feed flow rate of  $Q = 450 \text{ cm}^3 \text{ s}^{-1}$ , the corresponding output SS concentration,  $[conc]_{SF} = 0.00885 \text{ g L}^{-1}$  and risk failure,  $p_1 = 1.0$  with an assumed tolerance of 10 %. The table however shows only one of the 10,000 random samples in the Fr 13 simulations for SF.

A graphical summary of the distribution for the risk factor  $(p_1)$  is illustrated for all 10,000 scenarios for SF in Fig. 6.3. The computed value of risk factor  $p_1$  is the *x*-axis and the probability of  $p_1$  actually occurring (Vose, 2008) the *y*-axis. It can be noted the area under the curve is (~ 0.015 x 65 =) one (1). A total of 2,000 failures in the 10,000 samples were identified. These failures are highlighted in the R side of the figure. The failure rate is therefore 20 %, averaged over an extended period of time.



**Fig. 6.3:** Distribution for the risk factor ( $p_1$ ) from 10,000 scenarios of rapid sand-filtration (SF). All  $p_1 > 0$  highlight a failure.

Importantly, a log reduction  $\log_{10} [conc]_{SF} / [conc]_{SF0} - 1.11$  was found for SF. This is a ~ 90% reduction in the rapid SF.

In Table 6.4, 10 selected failures from the 2,000 in 10,000 scenarios for SS particle removal in SF are presented. A major benefit of presenting results in this way is that they

can be readily used to identify the value of each of the key parameters that in combination resulted in a failure (Zou and Davey, 2016; Abdul-Halim and Davey, 2016). For example, column 5, failure 4 (**bolded text**), shows that with input SS concentration [*conc*]<sub>SF0</sub> = 0.100 g L<sup>-1</sup> and feed flow rate of Q= 456 cm<sup>3</sup> s<sup>-1</sup>, yields an output SS concentration [*conc*]<sub>SF</sub> = 0.00788 g L<sup>-1</sup>, with risk factor  $p_I$  = 1.0 - showing a failure in SF. This is the particular scenario reported in Table 6.3.

With these 2,000 failures in SF as the input SS concentration to the UV reactor  $([conc]_{SF} = [conc]_{SF-UV})$ , some 4,041 UV reactor failures were identified with a 10 % tolerance. That is, an overall underlying failure rate of (4,041/10,000 =) 40.4 % is established for the two-step SF-UV. Simulations for UV reactor using the corresponding  $[conc]_{SF-UV}$  revealed a 3-log<sub>10</sub> reduction in viable *E. coli*.

Table 6.5 presents the corresponding output scenarios in the annular UV reactor with the 10 failures in SF from Table 6.4 as inputs. The table reveals five (5) of the 10 corresponding scenarios had failed operations, as highlighted by  $p_2 > 0$  in column 2, 5, 6, 7 and 9, corresponding to failure numbers 1, 4, 5, 6 and 8. **Table 6.4:** Ten (10) selected *Fr 13* failures from 2,000 in 10,000 scenarios for SS removal in SF with a 10 % tolerance. (The**bolded text** of column 5, failure 4, is the particular scenario shown in Table 6.3).

Parameters	10 selected SF Fr 13 failures									
	1	2	3	4	5	6	7	8	9	10
$[conc]_{SF0} (g L^{-1})$	0.101	0.102	0.107	0.100	0.096	0.099	0.097	0.099	0.104	0.095
$Q (\text{cm}^3 \text{ s}^{-1})$	456	453	439	456	466	457	455	458	445	441
$[conc]_{SF}(g L^{-1})$	0.00795	0.00793	0.00790	0.00788	0.00788	0.00786	0.00760	0.00784	0.00785	0.00703
$p_1$	0.17	0.40	0.70	1.00*	1.02	1.17	4.15	1.40	1.37	10.57

\* Values are reproduced as exactly those from r-MC sampling; it is not implied they need to be measured in this order.

**Table 6.5:** Corresponding output scenarios for UV reactor with the 10 failures in SF of Table 6.4 as inputs with 10 % tolerance.(The **bolded text** of column 5, failure 4, is the particular scenario shown in Table 6.3).

Parameters		10 selected UV Fr 13 scenarios								
	1	2	3	<b>4</b> <sup>†</sup>	5	6	7	8	9	10
$Q (\rm{cm}^3 \rm{s}^{-1})$	456	453	439	456	466	457	455	458	445	441
$[conc]_{SF-UV}(g L^{-1})$	0.00795	0.00793	0.00790	0.00788	0.00788	0.00786	0.00760	0.00784	0.00785	0.00703
$\ln N/N_0$	-5.72	-6.18	-9.05	-5.75	-4.52	-5.63	-5.96	-5.54	-7.66	-8.65
$\log_{10} N/N_0$	-2.48	-2.68	-3.93	-2.50	-1.96	-2.45	-2.59	-2.41	-3.33	-3.75
<i>p</i> <sub>2</sub>	0.80	-6.41	-51.08	0.33	19.59	2.19	-2.89	3.59	-29.40	-44.81

<sup>†</sup> Values shown are computed from r-MC sampling; it is not implied they need to be measured to this order.

#### 6.6. Discussion

#### 6.6.1. SF-UV global model

The computations for the Fr 13 global risk assessment proved to be stable, and because careful checks showed the mean simulation outputs agreed with the SVA, it was concluded that there were no computational and programmable errors in the computations.

If each scenario of the integrated SF-UV can be considered a daily continuous operation, then on average there would be (4,040/10,000 days x 365.25 days/year =), 148 failures each year to meet the required Regulatory reduction of  $4 - \log_{10}$  (Das, 2001) in viable *E. coli* due to within-system, stochastic effects. These failures however are not expected to be spaced equally in time.

For integrated SF-UV the *Fr 13* simulations revealed that for potable water production in an annular UV reactor the operation is actually a mix of successful and failed operations. Importantly however, as can be seen from Table 6.5 not all failed scenarios from SF automatically lead to a failure in the sequential UV reactor.

Ten (10) selected scenarios were selected from the *Fr 13* risk assessment for the sequential SF-UV global model, Table 6.6. For example, the **bolded text** in column 5, scenario 4, demonstrated that for SF with input  $[conc]_{SF0} = 0.100 \text{ g L}^{-1}$  together with  $Q = 456 \text{ cm}^3 \text{ s}^{-1}$  reduced the output  $[conc]_{SF-UV} = 0.00788 \text{ g L}^{-1}$  and resulted in  $p_1 = 1.00$  with a 10 % tolerance. With  $[conc]_{SF-UV} = 0.00788 \text{ g L}^{-1}$  as the input concentration to UV irradiation, yielded the average water velocity in the UV annular reactor gap  $v = 95.08 \text{ cm s}^{-1}$ , bulk residence (exposure) time  $\tau = 2.1 \text{ s}$ , UV dose  $[dose] = 114,313 \text{ }\mu\text{W} \text{ s cm}^{-2}$ , inactivation

constant  $k = 3.30 \text{ mW}^{-1} \text{ s}^{-1} \text{ cm}^2$ , Reynolds number, Re = 10,510 (dimensionless), friction factor for the UV reactor f = 0.0078 and the boundary layer thickness  $\delta = 238.87$  cm. Giving therefore the reduction in contaminant viable *E. coli* ln *N*/*N*<sub>0</sub> = -5.75 and log reduction log<sub>10</sub> *N*/*N*<sub>0</sub> = -2.50 resulting in the failure factor of  $p_2 = 0.33$ .

Other failed scenarios, for example, are 1, 4, 5, 6 and 8. Other scenarios i.e. 2, 3, 7, 9 and 10 can reasonably considered successful two-steps SF-UV operations to remove viable *E. coli* for potable water production because the sequential SF-UV operations are  $p_2 < 0$ .

	Fr 13 scenario									
	1	2	3	4	5	6	7	8	9	10
<u>SF</u>										
$[conc]_{SF0} (g L^{-1})$	0.101	0.102	0.107	0.100	0.096	0.099	0.097	0.099	0.104	0.095
$Q(\text{cm}^3 \text{ s}^{-1})$	456	453	439	456	466	457	455	458	445	441
$[conc]_{SF-UV}(g L^{-1})$	0.00795	0.00793	0.00790	0.00788	0.00788	0.00786	0.00760	0.00784	0.00785	0.00703
$p_1$	0.17	0.40	0.70	1.00	1.02	1.17	4.15	1.40	1.37	10.57
UV reactor										
$v ({\rm cm  s^{-1}})$	95.13	94.48	91.53	95.08	97.19	95.26	94.79	95.40	92.79	91.87
$\tau(s)$	2.1	2.1	2.1	2.1	2.1	2.1	2.1	2.1	2.1	2.1
[dose] (µW s cm <sup>-2</sup> )	114261	115041	118750	114313	111832	114101	114666	113938	117147	118311
$k (\mathrm{mW}^{-1}\mathrm{s}^{-1}\mathrm{cm}^2)$	3.28	3.52	4.94	3.30	2.66	3.23	3.40	3.19	4.26	4.75
Re (dimensionless)	10515	10443	10117	10510	10743	10529	10477	10544	10256	10155
f (dimensionless)	0.0078	0.0078	0.0079	0.0078	0.0078	0.0078	0.0078	0.0078	0.0079	0.0079
$\delta$ (cm)	238.89	238.49	236.60	238.87	240.18	238.98	238.68	239.06	237.41	236.82
$\ln N/N_0$	-5.72	-6.18	-9.05	-5.75	-4.52	-5.63	-5.96	-5.54	-7.66	-8.65
$\log_{10} N/N_0$	-2.48	-2.68	-3.93	-2.50	-1.96	-2.45	-2.59	-2.41	-3.33	-3.75
$p_2$	0.80	-6.41	-51.08	0.33	19.59	2.19	-2.89	3.59	-29.40	-44.81

# Table 6.6: Ten (10) selected Fr 13 scenarios of the global SF-UV demonstrated with E. coli.

The summary of the 10 selected *Fr 13* scenarios of Table 6.6 for the combined SF-UV model is presented visually as Table 6.7, shown as F = Fail and NF = Not Fail. It can be pointed out in the table, row 4, that five (5) of the 10 scenarios were failed scenarios for the integrated SF-UV process. Importantly, this visual display provides insights of the random nature of *Fr 13* failure and the impact of the naturally random fluctuations in key parameters in overall SF-UV global model.

**Table 6.7:** Visual summary of the 10 selected *Fr 13* scenarios of Table 6.6 for the combined SF-UV global model demonstrated with *E. coli* with a 10 % tolerance.

OperationFr 13 scenario										
	1	2	3	4	5	6	7	8	9	10
SF	F	F	F	F	F	F	F	F	F	F
SF-UV	F	NF	NF	F	F	F	NF	F	NF	NF

F = Failure NF = Not Failure

The significance of this methodology is that the insight is not available from other traditional risk analyses because the random (stochastic) part is not usually explicit in these. The distribution of the 10,000 scenarios for risk factor ( $p_2$ ) is shown in Fig. 6.4. The figure illustrates the combined failed and successful operations of the sequential SF-UV for the removal of viable *E. coli* in potable water production. It is important to note that these failures do not need 'faulty fittings' or 'human errors' to be invoked as explanation (Cerf and Davey,

2003). They are due to the impact of natural occurring (stochastic) fluctuations within the integrated SF-UV.



**Fig. 6.4:** Distribution for the risk factor ( $p_2$ ) from 10,000 scenarios of the sequential SF-UV operations, where  $p_2 > 0$  is a failure.

The Spearman rank correlation coefficient (Snedecor and Cochran, 1989) can be used to quantify the individual impact of key parameters in overall SF-UV efficacy, Table 6.8. This is readily available in @*Risk*. The table reveals there is a strong correlation (+0.70) between the volumetric flow rate of water (Q, cm<sup>3</sup> s<sup>-1</sup>) and  $p_2$ , and a strong inverse correlation (-0.69) with the lamp intensity ( $I_0$ ,  $\mu$ W cm<sup>-2</sup>). There is a weak correlation (+0.03) between the SS concentration ([*conc*]<sub>SF-UV</sub> g L<sup>-1</sup>) and  $p_2$ . This was highlighted by Abdul-Halim and Davey

(2016), where they unexpectedly discovered that although initially there was a highly significant loss of UV efficacy due to SS, the naturally occurring random fluctuation around the mean concentration of SS in feed water is not meaningfully impacting UV efficacy and vulnerability to survival of numbers of unwanted viable *E. coli*. It can be concluded that the controlling parameters in sequential SF-UV process are the natural fluctuations in feed-water flow (Q) together with fluctuations in lamp intensity ( $I_0$ ).

**Table 6.8:** Spearman rank correlation coefficient (Snedecor and Cochran, 1989) for the key input parameters on risk factor ( $p_2$ ) in the global SF-UV model.

Input parameter	Coefficient
$Q (\mathrm{mL s}^{-1})$	+0.70
$I_0 (\mu { m W} { m cm}^{-2})$	- 0.69
$[conc]_{SF-UV}$ (g L <sup>-1</sup> )	+0.03

#### 6.6.2. Presentation of risk results

As highlighted in the Blackett Review (Anon., 2012), typically presentation of risk data can present challenges. In this paper, the presentation of risk results is based on developing methodology of Davey and co-workers (e.g. Chandrakash and Davey, 2017; Zou and Davey, 2016; Abdul-Halim and Davey, 2015; 2016; Davey, 2015; Chandrakash et al., 2015; Patil et al., 2005) where the risk factor (*p*) permits ready identification and sorting of all

failure / non-failure scenarios in standard spread sheeting accessible by a wide range of users. Tabulated presentations are used to readily reveal and identify each parameter combination that leads to failure. This is important to gain insight into behavior of physical plant parameters control, and possible need for re-designs or changed controls in second-tier study (Chandrakash et al., 2015).

#### 6.6.3. Efficacy of integrated SF-UV

Abdul-Halim and Davey (2016) suggested that removal of SS prior to UV inactivation would increase UV efficacy in overall SF-UV water treatment process. Based on the results, there is notably a highly significant increase in UV efficacy in the annular reactor from the  $log_{10} = -0.92$  reported by Abdul-Halim and Davey (2016) due to the presence of UV shielding agent.

The reduction of SS in water after filtration process with SF was  $log_{10}$  -1.11 (~ 90 % removal). Subsequently, the overall removal of pathogens for potable water production was  $log_{10} = -2.93$  (99.9 % removal) after UV inactivation process.

This finding agrees well with that reported by Rajala et al. (2003) who showed experimentally that the concentration of SS can be reduced by about 90% (1-log<sub>10</sub> reduction) whilst further treatment with UV irradiation can further reduced the number of pathogens by 99.9% (3-log<sub>10</sub> reduction). SF with subsequent UV irradiation has proved to reduce the number of pathogens to a low level, often below the detection limit (Rajala et al., 2003). This is because the micro-organisms are not inhibited by SS that prevent UV light from penetrating to inactivate pathogens, thereby increasing efficacy. Notably, this reduction in viable pathogens is below Regulatory guidelines for potable water production of a minimum of 4-log<sub>10</sub> (99.99 %) reduction (Sommer et al., 2008).

It is concluded that the integrated SF-UV multiple-barrier (Betancourt and Rose, 2004) reduced levels of the viable pathogens greater than that obtained with exclusive use of standalone UV reactor.

However as this reduction falls below the Regulatory  $\log_{10} 4$  it is concluded that there is a need for pre-treatment with flocculation and sedimentation prior to SF to reduce the SS presence in feed-waters and therefore overall efficacy for potable water production in an annular UV reactor.

#### 6.6.4. Fr 13 and second-tier simulations

Importantly,  $Fr \ 13$  risk assessment offers new insight and a new possible analytical tool for risk simulations because  $Fr \ 13$  permits test re-designs and likely outcomes of targeted strategies in second-tier studies in synthesis and analysis. Second-tier studies is the effect of randomness not dependent on the process, therefore not reducible through further study; vulnerability to  $Fr \ 13$  only reduced by physical changes to system.

The impact of particular physical changes to system can be simulated through a judicial selection and testing of the probability distribution. This is because the system physical changes are mimicked by changes to the input distributions describing the key parameters.

For steady-state SF-UV, improved safety and reduced impact of naturally occurring fluctuations in key parameters on removal of pathogenic *E. coli* in potable water can be

achieved by specifying an increase in the safety tolerance (%*tolerance*) through repeat simulations in  $p_2$ . The significance of using %*tolerance* is to ensure the minimum design criteria or number or viable *E. coli* in the treated water is met. Repeat simulations are graphically summarized in Fig. 6.5.



**Fig. 6.5:** Impact of *%tolerance* on the number of overall integrated SF-UV failures ( $p_2$ ) per 10,000 scenarios.

The figure illustrates the impact of *%tolerance* on *Fr 13* failure of the integrated SF-UV operation ( $p_2$ ) per 10,000 scenarios for a range from  $2 \le \%$ tolerance  $\le 30$ . As is shown, by increasing *%tolerance*, the number of overall SF-UV failures decrease exponentially. With decreasing *%tolerance*, these failures greatly increase.

This result is interpreted as the greater the tolerance the greater the loss of flexibility and the greater the precision is needed for process control of the integrated SF-UV. This suggests that precision control of SF-UV reactor is beneficial to minimize vulnerability of these unexpected failures.

#### 6.6.5. Improving integrated SF-UV

Pre-treatment of the raw feed-water using coagulation/flocculation prior to SF could be undertaken to reduce the concentration of SS in the feed-water prior to the UV reactor.

Importantly, an improved feed-water control to limit naturally occurring fluctuations in flow could be used to improve overall efficacy of the treatment in the integrated SF-UV. As highlighted by Abdul-Halim and Davey (2016), the controlling parameter that has greatest impact on vulnerability to failure and unwanted survival of *E. coli* is the natural fluctuations in feed-water flow, together in combination with fluctuations in UV lamp intensity.

Alternatively, a slow sand-filtration could be used to obtain improved efficacy in sequential SF-UV operations (Ray and Jain, 2011). This is because slow sand-filtration does not usually require any pre-treatment process.

#### 6.7. Conclusions

Application of the *Fr 13* risk framework to a two-step integrated SF-UV for the first time for the production of potable water has shown an underlying vulnerability of 40.4 % to the unwanted survival of viable *E. coli*. This translates to 148 surprise failures per annum,

averaged over the long term. This new insight cannot be obtained from alternate risk and hazard assessments.

The mean reduction of SS in SF was  $log_{10}$  -1.11 (90 %), with a subsequent reduction of viable *E. coli* in the UV reactor of  $log_{10}$  -2.93 (99.9 %). This is a highly significant increase in UV efficacy compared with that ( $log_{10}$  -0.92) without pre-treatment of the raw feed in a standalone UV reactor, and underscores the utility of the integrated SF-UV.

Integrated SF-UV is actually a mix of successful and failed operations. Importantly, not all failed SF automatically result in failure in overall SF-UV process efficacy.

These findings will be of immediate interest to risk analysts, and benefit to operators and managers responsible for the production of potable water using UV irradiation.

## Nomenclature

The number in parentheses after description is the equation in which the symbol is defined or first used.

Α	Cross-sectional area of filter bed, $cm^2$ (6.7) and (6.8)
С	Correction constant for real reactor, $0.0125 \text{ cm} (6.15)$
Ci	Model coefficients (6.13)
[conc] <sub>SF</sub>	Suspended solids concentration in filter effluent, g $L^{-1}$ (6.1), (6.12) and (6.24)
[conc] <sub>SF0</sub>	Suspended solids concentration in filter influent, g $L^{-1}$ (6.1) and (6.12)
[conc] <sub>SF-UV</sub>	Suspended solids concentration in SF-UV influent, g $L^{-1}$ (6.13)
d	Annular gap width UV reactor, cm $(6.15)$ , $(6.20)$ and $(6.23)$
dc	Collector diameter, cm $(6.1)$ and $(6.4)$
dp	Particle diameter, cm (6.4), (6.6), (6.10) and (6.11)
[dose]	UV dose, $\mu$ W s cm <sup>-2</sup> (6.13) and (6.14)
f	Friction factor, dimensionless $(6.21)$ and $(6.22)$
g	Gravitational velocity, $cm^2 s^{-1}$ (6.6)
$I_0$	UV lamp intensity, $\mu$ W cm <sup>-2</sup> (6.14) and (6.15)
k	Inactivation constant, $\mu W^{-1} s^{-1} cm^2$ (6.13) and (6.15)
K <sub>B</sub>	Boltzmann constant, $1.381 \times 10^{-23} \text{ J K}^{-1}$ (6.10) and (6.11)
$L_{ m SF}$	Depth of sand-filter, cm $(6.1)$ and $(6.8)$
L	Length of radiation section, $cm (6.17)$

Ν	Concentration viable <i>E. coli</i> , $mL^{-1}$ (6.15), (6.16) and (6.25)
$N_{ m G}$	Gravity number, dimensionless (6.5) and (6.6)
$N_0$	Concentration viable <i>E. coli</i> before UV exposure, $mL^{-1}$ (6.15), (6.16) and
	(6.25)
$N_{\mathrm{R}}$	Relative size group, dimensionless $(6.3)$ and $(6.4)$
$p_1$	Failure risk factor for SF, dimensionless (6.24)
$p_2$	Failure risk factor for UV, dimensionless (6.25)
Pe	Peclet number, dimensionless (6.9) and (6.10)
Q	Volumetric flow rate, $\text{cm}^3 \text{ s}^{-1}$ (6.7) and (6.18)
$R_1$	Radius of inner cylinder of annular UV reactor, cm $(6.18)$ , $(6.19)$ and $(6.20)$
$R_2$	Radius of outer cylinder of annular UV reactor, cm (6.18), (6.19) and (6.20)
R <sub>c</sub>	Dimensionless group, $(6.15)$ and $(6.19)$
Re	Reynolds number, dimensionless (6.22) and (6.23)
Т	Temperature, K (6.10) and (6.11)
V	Average water velocity in UV annular gap, cm s <sup>-1</sup> (6.17), (6.18) and (6.23)
$V_{ m F}$	Filtration rate, cm s <sup>-1</sup> (6.6), (6.7), (6.10) and (6.11)
Vs	Stoke's settling velocity, cm $s^{-1}$ (6.6)
W	Width of SF, cm (6.8)

## Greek

α	Absorption coefficient, $\text{cm}^{-1}$ (6.15)
$\alpha_E$	Attachment efficiency, dimensionless (6.1)

δ	Boundary layer thickness UV reactor, cm $(6.15)$ and $(6.21)$
З	Porosity SF, dimensionless (6.1)
η	Total transport efficiency, dimensionless $(6.1)$ and $(6.2)$
$\eta_D$	Transport efficiency due to diffusion, dimensionless $(6.2)$ , $(6.9)$ and $(6.11)$
$\eta_G$	Transport efficiency due to gravity, dimensionless $(6.2)$ and $(6.5)$
$\eta_I$	Transport efficiency due to interception, dimensionless $(6.2)$ and $(6.3)$
$ ho_p$	Particle density, kg cm <sup>-3</sup> $(6.6)$
$ ho_w$	Feed water density at 20 $^{\circ}$ C, kg cm <sup>-3</sup> (6.6) and (6.21)
τ	Residence (exposure) time in UV reactor, s $(6.14)$ and $(6.15)$
μ	Dynamic viscosity of water, kg cm <sup><math>-1</math></sup> s <sup><math>-1</math></sup> (6.10), (6.11) and (6.21)
υ	Kinematic viscosity of water at 20 $^{\circ}$ C, cm <sup>2</sup> s <sup>-1</sup> (6.21)

### Other

SF	Rapid sand-filter
SS	Suspended solids
stdev	Standard deviation
UV	Ultraviolet irradiation reactor
%tolerance	practical tolerance (margin) in reduction in viable <i>E. coli</i> , $\%$ (6.24) and (6.25)

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**CHAPTER SEVEN** 

# CONCLUSIONS AND FUTURE DEVELOPMENT

#### 7.1. Conclusions

- 1. Steady-state processing is used globally in chemical engineering. Importantly however, there are naturally occurring random (stochastic) fluctuations in process parameters about a 'set' mean value. These are not sufficient to be considered transient, and, generally, a change in one is off-set by another with plant output behaviour seemingly steady. Significantly, these naturally occurring fluctuations are not addressed explicitly in traditional chemical engineering. However, Davey and co-workers have shown that these naturally occurring fluctuations can combine and accumulate in one direction and leverage unexpected (surprise) behaviour across a 'failure not failure' boundary. Their hypothesis they titled *Fr 13* to underscore the surprise element of the failure event. Significantly, the *Fr 13* risk framework is predicated on established unit-operations principles in chemical engineering. It is an advance over alternative assessments because it produces all possible plant behaviour outputs, including failures
  - 2. To improve present understanding of the vulnerability to failure of UV reactor irradiation for potable water production, the probabilistic *Fr 13* risk framework was applied for the first time. The overarching aim was to investigate how random fluctuations in apparent steady-state UV reactor parameters could be transmitted and impact efficacy of treatment. Failure was defined as unwanted levels of viable pathogenic *Escherichia coli* in the treated water a widely used indicator of public health risk. Importantly, steady-state ultraviolet (UV) irradiation for potable water production is becoming an important global alternative to traditional disinfection

192

by chlorination, especially in Asia. A failure of UV to reduce viable pathogens can lead to enduring health legacies, with or without fatalities

- 3. *Fr 13* predictions from a preliminary one-step analysis of a standalone annular UV reactor, that was synthesized for both simplified steady-state laminar flow and turbulent feed-water flow, showed a vulnerability to surprise failure of 0.4 % and 16 %, respectively, with an assumed practical tolerance (safety margin) of 10 % based on cumulative impact of stochastic (random) effects from naturally occurring fluctuations in feed-water flow and UV lamp intensity. These rates are averaged over the long term, and failures in the apparent continuous successful reactor would not be expected to be spaced-equally in time. Although this was a new insight into efficacy of UV irradiation for potable water, it was acknowledged a drawback however was that the underlying unit-operations was simplified
- 4. To test further the applicability and benefits of the *Fr 13* risk framework, a practically more realistic UV reactor model with suspended solids (SS) in the raw feed-water, that could act as both UV shielding and UV absorbing agents, was synthesized. Simulations of the impact of naturally occurring fluctuation in concentration of these solids in combination with those in lamp intensity (*I*<sub>0</sub>) and feed-water flow (*Q*) resulted in, respectively, some 32.1 % and 43.7 % vulnerability to failure to reduce the level of unwanted viable *E. coli* (ATCC 25922 'Seattle' strain) in the treated water over the long term. The efficacy of the UV reactor with solids in the raw-feed water was reduced to 1-log<sub>10</sub> reduction, compared with a 4.35-log<sub>10</sub> reduction without solids present. An unexpected finding was that UV vulnerability to failure with unwanted survival of pathogens is

impacted highly significantly by fluctuations in feed-water flow, but not those in concentration of solids. It was the initial presence of solids that reduced the practically achievable reduction in pathogenic viable *E. coli* in the annular UV reactor for potable water production. It was concluded therefore that pre-treatment of the feed-water was needed to exploit these findings to remove solids and to improve control of the feed-water flow to reduce the impact on efficacy of treatment of the water in the annular UV reactor

5. In consequence, a two-step *Fr 13* risk assessment of a sequential and integrated rapid sand-filter (SF) and annular UV reactor (SF-UV) was synthesized for the first time for potable water production. Simulations highlighted that apparent steady-state SF-UV is actually a mix of successful operations together with unsuccessful ones. For single-step SF, a vulnerability to failure to reduce levels of solids in the raw feed-water 20 % was revealed. When integrated as SF-UV, *Fr 13* simulations with a tolerance (safety margin) of 10 % highlighted a vulnerability overall of UV efficacy for potable water production of some 40.4 % of all continuous operations, averaged over the long term. The mean reduction of suspended solids in the SF treated feed-water was a 1-log<sub>10</sub> reduction (90 % removal). Subsequently, the in the overall SF-UV there was 3- log<sub>10</sub> reduction (99.9 %) in viable pathogens. This was because solids that inhibited UV light from penetrating to the pathogens had been removed in the SF. However, because the Regulatory standard for potable water requires a 4-log<sub>10</sub> reduction in viable *E. coli*, it was concluded that flocculation and sedimentation steps prior to SF should be investigated

- 6. Importantly, this research has highlighted the fact that that apparent steady-state continuous UV irradiation for potable water production is a combination of successful and failed operations. This insight is new and cannot be obtained using traditional risk and hazard approaches, with or without sensitivity analyses
  - 7. Second-tier simulation studies available with the *Fr 13* framework underscored that reduced vulnerability to UV failures could be practically achieved by installing improved process control on the raw feed-water, and; by regular and continuous monitoring of suspended solids in the feed-water. To confirm these *Fr 13* predictions for the UV annular reactor and integrated SF-UV, process validation trials with experimentally determined new data are needed. However this is beyond the scope of the present work
- 8. It is concluded that the *Fr 13* framework appears generalizable to a range of microorganism contaminants in the raw feed-water, and; to generic steady-state UV processing with increasing complexity and interconnectedness beyond SF-UV to involve flocculation and sedimentation steps. There is no evidence of methodological barriers to advancement. If properly developed, the *Fr 13* framework could provide a new process design tool that could be adapted at both synthesis and analysis stages to provide new insight and knowledge about UV irradiation and related process plant behaviour
- 9. Findings from this research work will aid a detailed understanding of the factors that could contribute to unexpected failures, and will result in increased confidence in steady-state processing of (bio) chemical engineering unit-operations.

This research work is original and not incremental work. Results obtained from this research will benefit risk researchers, water processors and designers of UV reactors.

#### 7.2. Future development

Importantly, the success of this research shows that the Fr 13 risk framework can, in principle, be applied to minimize risk and vulnerability to failure in a range of steady-state processes of increasing complexity and inter-connectedness. Whilst this research has demonstrated efficacy of UV irradiation for potable water production, opportunities for extending the research remain. This section presents some of these:

#### 1. <u>Multi-step UV irradiation processing for potable water</u>

Based on the methods demonstrated in this thesis, there is an opportunity to develop and advance the *Fr 13* framework to multi-step unit-operations for UV potable water production. For example, Fig. 7.1 shows a 3-step sequential and integrated sedimentation, filtration and UV irradiation, or, more broadly, 4-steps with integrated coagulation/flocculation, sedimentation, and filtration and UV irradiation. This work would lead to an optimization of safety with reduced risk of failure to reduce unwanted levels of viable pathogens in treated water.


Fig. 7.1: Multi-step unit-operation processes in potable water production.Highlighted is the future work that can be developed for *Fr 13* risk framework.

## 2. <u>A generic process</u>

Because of the general success of the *Fr 13* framework, and reinforced in this research, it is planned to apply it to a generic process (Davey, 2017)<sup>1</sup>. A generic process is considered to involve each of at least one feed(s) stream, reactor, separator, recycle and purge, stream. Preliminary results reveal a counter-intuitive depiction of apparent steady-state processing

## 3. <u>Coupling with chemical engineering commercial software</u>

In the longer term Fr 13 has the potential to be coupled with commercial chemical engineering design software such as ASPEN Plus<sup>®</sup> and Batch Process Developer<sup>®</sup>. This will produce more powerful design and assessment tools to improve process outcomes in the foods and chemical industries.

<sup>&</sup>lt;sup>1</sup> Davey, K.R. 2017. Failure modelling of a generic process with feed-stream, reactor, separator and recycle with purge – A Friday 13<sup>th</sup> risk assessment. *Chemical Engineering Science* – in preparation.

## A Definition of Some Important Terms used in this Research

E. coli	<i>Escherichia coli</i> is a gram-negative, facultatively anaerobic, rod-shaped, coliform bacterium that is commonly found in the lower intestine of warm-blooded organisms (Amos, 2007). <i>E. coli</i> is pathogenic species of bacteria widely used as an indicator of health risk.		
Failure	This is defined as the failure of UV irradiation to reduce viable numbers of the pathogen <i>Escherichia coli</i> in the treated water		
Failure modeling	Structured risk technology based on established unit-operation used to estimate and analyze the likelihood of unexpected failures in steady-state unit-operation and process		
Friday 13th syndrome	Event defined where adverse outcomes combine to result a failure of plans and opportunities despite all good design and operation as defined by Davey and Cerf (2003)		
Fr 13 simulation	Novel, probabilistic simulation for a predicted model output with probability distribution of values as inputs (developed b Davey and Cerf (2003))		
Probability	A numeric measure of the likelihood of a particular outcome a stochastic process scenario		
r-MC	refined-Monte Carlo simulation		
Single Value Assessment	Traditional, deterministic model solution for a predicted model output with single value inputs as defined by Davey and Cerf (2003) and Sinnott (2005)		
Uncertainty	Lack of knowledge, or level of ignorance about parameters that characterize the physical or process system being modelled. Uncertainty is sometimes reducible through further measurement, carefully study, or consulting more experts (Vose, 2008)		
Unit-operation	A basic step in process involving physical change or chemica transformation taking place e.g. separation, evaporation, heating, distillation, etc		
Variability	The effect of chance and a function of the system. Variability is not reducible through either further measurement or study, but might be reduced by changing or controlling the physical system (Vose, 2008)		

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## Friday 13<sup>th</sup> Failure Modelling: A New Quantitative Risk Assessment of UV Irradiation for Potable Water

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## FRIDAY 13<sup>TH</sup> FAILURE MODELLING: A NEW QUANTITATIVE RISK ASSESSMENT OF UV IRRADIATION FOR POTABLE WATER

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## ABSTRACT

UV irradiation is an alternative to widely used chemical disinfection to produce potable water. Failure of a well-run, well-maintained UV plant can lead to catastrophic and enduring public health effects, with or without fatalities. Failure is defined as the unexpected survival of levels of pathogenic Escherichia coli. Friday 13th failure modelling (Fr 13) is an emerging method for new quantitative risk assessments of unexpected failure in process plant due to "within system" chance (stochastic) changes. In this original research a new Fr 13 risk assessment of a simplified unit-operations model for UV irradiation for potable water is presented for the first time. A comparison is made between the predictions from a traditional, single point assessment and Fr 13 model using established UV inactivation kinetics for E. coli. A process risk factor (p) is synthesised in the Fr 13 model and is solved using a refined Monte Carlo simulation with Latin Hypercube sampling. Results reveal that 47 in every 10,000 continuous UV operations can fail unexpectedly with a tolerance of 10% on the design level of reduction in E. coli. This translates, on average, to an unexpected survival of E. coli each 0.58 years of continuous operation. This new insight is not available from traditional assessments, with or without sensitivity analyses. Practical methods of reducing unexpected failure and improving process technology in UV plant for potable water are briefly discussed.

## INTRODUCTION

UV irradiation provides an alternative to widely used chemical disinfection to economically produce large volumes of potable water (Kim *et al.*, 2002). It is effective in the inactivation of both bacterial and viral contaminants. Other advantages include that it is non-intrusive, produces no noticeable adverse odour or taste (Kiely, 1998; Nguyen, 1999), has low energy and space requirements compared with chemical disinfection (Amos, 2007; Amos *et al.*, 2001), and is generally more cost effective (Kim *et al.*, 2002; Okpara *et al.*, 2011). The cost of UV irradiation has decreased over recent years due to improvements in lamps and plant designs (Okpara *et al.*, 2011).

Because failure of UV plant can lead to enduring public health effects, with or without fatalities, a quantitative understanding of process risk is important. Current risk assessment methods (Haas, 1983; Medema *et al.*, 2003; Okpara *et al.*, 2011; Regli *et al.*, 1991; Teunis *et* 

*al.*, 1997) however lack a sense of "process" and are semi-quantitative (Davey, 2010). Often a "risk" is reported when what is actually meant is a "hazard" (Davey, 2010).

Of emerging research interest is the notion that no matter how good the design and operation of process plant there will be an occasional, unexpected failure. This practically observable and widely acknowledged phenomenon in otherwise well-operated, well-maintained process plant has been titled *Friday 13<sup>th</sup> failure (Fr 13)* by Davey and co-workers (Cerf & Davey, 2001; Davey, 2011a, 2011b; Davey *et al.*, 2011). *Fr 13* is the result of an accumulation of small variations in key process parameters that combine in one direction to leverage unexpected changes in process conditions. Often "human error" or "faulty fittings" are falsely blamed (Cerf & Davey, 2001; Davey, 2001; Davey, 2010, 2011b; Langer, 2008).

The principal aim of this original research is to report for the first time a quantitative risk assessment of unexpected failure of UV irradiation for potable water using the new Fr 13 failure modelling. An advantage highlighted over traditional methods of Fr 13 is an enhanced understanding of risk in UV irradiation for potable water which can be used to safeguard plant and public health, and guide improved process technologies.

### A MODEL FOR UV IRRADIATION

An essential first step is the synthesis of an adequate unit-operations model for UV irradiation.

This requires a marriage and integration of equations for UV lamp intensity, residence time of the water to the lamp, and; kinetics of inactivation of water-borne contaminants. The criteria for an adequate model must include (Amos *et al.*, 2001):

- Accuracy of prediction against observed data
- Ease of synthesis and use i.e. relative complexity of *economy/elegance*
- A generalized form applicable to a wide range of micro-organisms.

UV dose is the key parameter. This can be calculated from exposure time of the water (t) to lamp intensity (I) (Amos, 2007; Amos *et al.*, 2001; Loge *et al.*, 1996) such that:

$$[dose] = It \tag{1}$$

where all symbols used are defined in the Notation at the end of this paper. The kinetics of UV inactivation are widely assumed to be a first-order reaction with respect to dose (Amos, 2007; Amos *et al.*, 2001; Hijnen *et al.*, 2006; Loge *et al.*, 1996). Mathematically this can be represented as:

$$\ln(\frac{N}{N_0}) = -kIt = -k[dose]$$
<sup>(2)</sup>

or conveniently to base log<sub>10</sub>:

$$\log_{10}(\frac{N}{N_0}) = \ln(\frac{N}{N_0})/2.303$$
(3)

From Equation (2) a plot of  $\ln (N/N_0)$  versus UV dose gives a straight-line through the origin with slope, k.

A widely used indicator pathogen in potable water production is *Escherichia coli* (Amos, 2007; Amos *et al.*, 2001).

Importantly, any suspended solids in the water will act as a shielding-agent to dose and will result in low UV efficacy (Amos *et al.*, 2001; Loge *et al.*, 1996; Nguyen, 1999). Amos *et al.* (2001) demonstrated the Davey-Linear Arrhenius equation to be the most adequate for description of UV irradiation of viable *E. coli* in comparison with the classical log-linear, Square-Root and  $n^{\text{th}}$  Order Polynomial models. This finding was based on extensive analyses of residual plots of experimental data and appropriate criteria including: parsimony and ease of use and ready integration with additional equations to describe a UV irradiation unit-operation.

The Davey-Linear Arrhenius for UV inactivation of *E. coli* in the presence of suspended solid is given by:

$$\ln k = C_0 + C_1 [dose] + C_2 [dose]^2 + C_3 [conc]$$
(4)

This equation is said to be "additive" in form i.e. [dose] and [conc] appear to act independently to effect inactivation (Amos, 2007; Daughtry et al., 1997). It is widely applied to general inactivation of micro-organisms (McMeekin et al., 1993; Bruin & Jongen, 2003; Min & Choi, 2009).

Equation (1) through (4) establishes the simplified unit-operations model for UV irradiation of E. *coli* for potable water.

## FRIDAY 13th FAILURE MODEL

### Defining UV Failure

An essential element of a Fr 13 quantitative risk assessment is a clear definition of a process (or product) risk factor, p (Davey, 2010, 2011b). A suitable risk factor for UV irradiation can be defined as the design  $\log_{10}$  reduction in viable E. *coli* together with an acceptable level of *%-tolerance* such that:

$$p = -\% tolerance + 100[1 - \frac{\log_{10}(\frac{N}{N_0})}{\log_{10}(\frac{N}{N_0})}]$$
(5)

where  $\log_{10}(\frac{N}{N_0})$  is an instantaneous value of  $\log_{10}(\frac{N}{N_0})$ . This is computationally convenient because as can readily be seen from Equation (5) for all p > 0 UV fails.

## Simulating Friday 13th

In simulation of a Fr 13 model key parameters are defined by a distribution of values, the mean of which generally agrees with the traditional single point, or single value assessment (SVA) (Cerf & Davey, 2001; Davey, 2011b; Patil, 2006; Patil *et al.*, 2005). The parameter distribution is carefully defined so as to cover all practical values that might occur in day-to-day operations (Cerf & Davey, 2001; Davey, 2010, 2011a, 2011b; Davey *et al.*, 2011; Patil, 2006). A refined Monte Carlo sampling is used with Latin Hypercube sampling to ensure that the random samples within each probability distribution cover the entire range of the

distribution (Davey, 2011b; Vose, 2008). To ensure the output distribution is *Normal* a minimum number of random samples are necessary; this usually means 1,000 to 50,000 samples will be needed (Davey K R - *unpublished data*). It is a simple matter to establish this visually with most software.

The "within system" practical variation (sdev) in the lamp intensity is assumed at 1% and for each of the concentration of shielding agent [conc] and residence time, t, 5%.

The selected distributions for *I*, [conc] and *t* are defined as: **RiskNormal**(mean, sdev, **RiskTruncate**(minimum = mean - 2\*sdev), (maximum = mean + 2\*sdev))). For example, for the lamp, this means a mean intensity of 11,940 with sdev of 120 and a minimum 11,700 and maximum 12,180  $\mu$ W cm<sup>-2</sup> is used. The distributions are truncated to indicate that the chance of a practical process value being outside the range is (zero) negligible. A practical process tolerance of 10% on the required log<sub>10</sub> reduction of viable *E. coli* is assumed.

Calculations were performed in Microsoft Excel<sup>TM</sup> with a commercially available add-on  $@Risk^{TM}$  (pronounced at-risk) version 5.7 (Palisade Corporation). This is convenient because Excel has nearly universal use, and therefore makes communication of results streamlined.

Simulations were used to identify practical process events that give rise to UV failure i.e. for all values of the risk factor p > 0.

## RESULTS

Table 1 presents a summary comparison of the Fr 13 and traditional single point (SVA) assessments for UV irradiation using the Davey Linear-Arrhenius kinetics for inactivation of viable *E. coli* in water with suspended solids, and a process tolerance of 10% on the design level of reduction. The UV process parameters are given in column 1 of the table. These are the lamp intensity, suspended solids concentration and residence time. Traditional SVA calculations are presented in column 2.

10,000 random samples of each input distribution (*I*, [conc] and t) were used. This means calculations will have been performed on all possible combinations of practical process scenarios that could occur in the UV unit-operation. The values in column 3 of the table are for one only scenario of these 10,000. For this scenario shown it can be seen that p > 0, indicating UV failure.

Table 1:	Comparison of traditional single point (SVA) and Fr 13 risk assessments for UV
	irradiation for potable water with the Davey Linear-Arrhenius equation
	for inactivation of E. coli

UV Parameter	SVA*	Fr 13*		
$I (\mu W cm^{-2})$	11940	11811.66895	RiskNormal(11940, 120, RiskTruncate( 11700, 12180))	
[conc] (gl <sup>-1</sup> )	0.115	0.11638	RiskNormal(0.115, 0.006, RiskTruncate( 0.104, 0.127))	
<i>t</i> (s)	1.90	1.71616	RiskNormal(1.9, 0.095, RiskTruncate( 1.710 2.090))	
[dose] (µWscm <sup>-2</sup> )	22686.00	20270.68555	Equation (1)	
$k (\mu W^{-1} s^{-1} cm^2)$	0.0004139	0.00041395	Equation (4)	
$\ln N/N_0$	-9.391	-8.39101	Equation (2)	
log10 N/No	-4.078	-3.64351	Equation (3)	
p		0.64672	Equation (5)	

\* SVA = Traditional single point, or, Single Value Assessment

\* With Latin Hypercube sampling

A total of 47 failures were identified in the 10,000 scenarios. Five of these are presented in Table 2 where it can be seen all have a value of p > 0. This table shows combinations of the practically realizable values of the UV process parameters that led to failure to achieve the design reduction in level of viable *E. coli* (with the assumed tolerance of 10%). In the table, row 2, shows the combination of randomly sampled values for, respectively, I = 11811.66895  $\mu$ Wcm<sup>-2</sup>, [conc] = 0.11638 g  $\Gamma^1$  and t = 1.71616 s, resulted in a corresponding value of p = 0.64672; this is the particular scenario given in Table 1.

Table 2: 5 failures from 47 in 10,000 UV irradiation scenarios

Ι	[conc]	t	р
(µWcm <sup>-2</sup> )	$(g l^{-1})$	(s)	
11741.15137	0.11916	1.71136	1.42826
11811.66895	0.11638	1.71616	0.64672
11740.73730	0.11451	1.73133	0.39807
11863.45508	0.11532	1.71656	0.23402
11890.02539	0.10521	1.71595	0.065038

### DISCUSSION

If each simulation scenario is thought of as an operational day, then an unexpected Fr 13 failure in UV irradiation would occur once every (10,000/365.25/47 =) 0.58 years on average despite best operation and maintenance. These would not, of course, be spaced equally in time.

As the process *%-tolerance* is increased the model can be used to show the number of failures will reduce, and conversely, increase with a reduced *%-tolerance*.

This implies a practical method of reducing Fr 13 failure in UV irradiation is to reduce the variance in key input parameters through improved process control. An apparent exponential dependence of failure rates suggests that increased costs for improved process control could be readily justified.

A practical question is how the value of the risk factor p will be affected through improved process control: the answer is, some experimenting will need to be done using the Fr 13 model. In more general situations knowledge from experienced operators or "experts" could be drawn on to devise a process-specific distribution (Davey, 2010, 2011b).

The general principle of Fr 13 modelling has been illustrated i.e. to calculate the combined impact of chance (variability) in key parameters on the probability distribution (likelihood) of possible process outcomes. Traditional SVA approaches, with or without a sensitivity analysis, do not separate these (Hoffman & Hammonds, 1994; Ria & Krewski, 1998) and therefore cannot give practical insight into unexpected UV failures. SVA estimates of risk may actually give a greater sense of process safety than is the case (Cerf & Davey, 2001; Davey, 2011b); this is tacitly acknowledged as many processes involve deliberate overtreatment which is wasteful not only in energy, but plant costs.

The valuable insight gained with Fr 13 risk modelling into UV irradiation for potable water over traditional methods has been to quantitatively identify fail scenarios that are probable. Importantly, Fr 13 can be used as a second-tier simulation to investigate any proposed physical changes to the process (Davey, 2011b).

## CONCLUSIONS

New Fr 13 quantitative risk model has revealed that failure of UV irradiation for potable water, defined by unwanted viable E. *coli* post-treatment, can result from chance (stochastic) variability in key process parameters. The number of failures is related to the combined effects of variance about process parameter mean values.

Reducing the variance in key parameters, through for example improved process control, whilst potentially costly, can minimize likelihood of UV failures.

Fr 13 modelling can be used to quantitatively assess reduced risk of UV failures from proposed changes in process control or design, or intervention strategies, and therefore can be used to guide improvements in process safety and technology. This is because Fr 13 modelling is a significant elaboration on current and limited SVA analyses as it produces all possible outcomes of UV operations.

## NOTATION

- *C<sub>i</sub>* Davey Linear-Arrhenius coefficients for UV shielding of *E. coli* (Amos, 2007):  $C_0 = -6.334; C_1 = -7.71 \ge 10^{-5}; C_2 = 7.23 \ge 10^{-10}; C_3 = -0.685$
- k rate coefficient for UV inactivation,  $\mu W^{-1} s^{-1} cm^2$
- N number of viable E. coli at t = t
- $N_0$  number of viable *E*. *coli* at t = zero
- [conc] solids (shielding) concentration,  $0.115 \text{ g l}^{-1}$
- [dose] UV dose, I t,  $\mu$ W s cm<sup>-2</sup>
- I UV lamp intensity, 11,940  $\mu$ W cm<sup>-2</sup>
- t exposure time, 1.9 s
- *p* risk factor, dimensionless

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## A Friday 13th Risk Assessment of Failure of Ultraviolet Irradiation for Potable Water in Turbulent Flow

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## A Friday 13th risk assessment of failure of ultraviolet irradiation for potable water in turbulent flow



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### ABSTRACT

Ultraviolet (UV) irradiation for potable water is an important alternative to widespread disinfection methods such as chlorine. Failure of UV irradiation to reduce levels of viable contaminants can lead to enduring health effects, with or without fatalities. Here a new risk assessment of failure of UV irradiation for potable water in turbulent flow in a series annular-reactor is presented using the Friday 13th (*Fr* 13) methodology of Davey and co-workers (*Food Control* 29(1), 248–254, 2013). The aim was to demonstrate the effects of random changes in UV parameters on plant failure. Failure is defined as unexpected levels of survival of *Escherichia coli*, a species of faccal bacteria widely used as an indicator for health risk. The assessment is based on a unit-operations model of UV irradiation together with extensive experimental data of Ye (2007). A failure factor (*p*) is defined in terms of the design reduction and actual reduction in viable *E. coli* contaminants. UV irradiation 15% of apparent successful operations, over the long term, can fail to achieve the design reduction in viable *E. coli* of 10<sup>-435</sup> due to random effects. The analysis is shown to be an advance on current risk assessments because it produces all possible practical UV outcomes. Implications of *Fr* 13 methodology for practical re-design and targeted physical changes to UV plant for improved reliability and safety is discussed.

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#### 1. Introduction

Ultraviolet (UV) irradiation for production of potable water is an increasingly attractive alternative to widely used chemical disinfectants, such as chlorine (Amos, Davey, & Thomas, 2001). Advantages of UV irradiation include that it: adds nothing to the water (compared to chemical disinfection); inactivates both bacterial and viral contaminants; produces no harmful by-products; does not alter the taste or properties of the water, and; is increasingly cost effective (Amos et al., 2001; Okpara, Oparaku, & Ibeto, 2011). Because of these advantages UV irradiation is increasingly relied on globally to produce potable water, and is often required to be in continuous operation for prolonged periods. Failure of UV irradiation to reduce viable contaminants to a safe level can lead to enduring public health effects, with or without fatalities. A quantitative risk understanding of UV irradiation plant is therefore important.

In recent years Davey and co-workers (Davey, 2010, 2011; Davey, Abdul Halim, & Lewis, 2012; Davey, Chandrakash, & O'Neill, 2011,

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2013; Patil, Davey, & Daughtry, 2005) have illustrated a novel risk assessment titled *Friday 13th (Fr 13)*. The idea is based on the practical notion that despite best design and operation of a continuous process there will be an occasional, unexpected and surprise failure that cannot be attributed to human error or faulty fittings (Cerf & Davey, 2001). A key insight is that an accumulation of random changes in otherwise well-operated continuous plant parameters can lead unexpectedly in one-direction and leverage significant sudden change in process or product. Published case studies include a sudden and unexpected change from sterile milk to non-sterile product (Davey & Cerf, 2003); from stable to unstable operation with fermenter "washout" (Patil et al., 2005); from clean to unclean (CIP) processing (Davey et al., 2011); and more generally, from safe to unsafe (Davey et al., 2012).

Current food safety management tools and alternative risk assessments include Microbiological risk assessment (Codex Alimentarius Commission CAC, 1998), HACCP (Hazard Analysis Critical Control Point), HAZOP (HAZard and OPerability) and Reliability Engineering (O'Connor, Newton, & Bromley, 2002). Importantly, although these methods have been adapted widely they cannot be used to understand and reduce random effects, with either more study or measurement (Anderson & Hattis, 1999; Vose, 2008). This is

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because this critical parameter in these assessments is omitted, or more strictly, "hidden". This is true also of the recent assessment of Riverol and Pilipovik (2014) who addressed process "failure frequency" with a case study on milk pasteurization. The assessment is not developed from widely used unit-operations principles in foods processing (see for example Foust, Wenzel, Clump, Maus, & Anderson, 1980; Ozilgen, 1998; Schwartzberg & Rao, 1990) and does not appear to be generalizable; it has much in common with *Reliability Engineering*. In contrast, an advantage with *Fr* 13 assessments is that both the facts about the process and the effects of random changes in parameters are separated (Davey et al., 2012, 2013; Hoffman & Hammonds, 1994; Ria & Krewski, 1998). This is more mathematically correct and permits the effect of each to be studied.

The principle of *Fr* 13 is that it is predicated on the underlying unit-operations model together with a practical definition of product failure and a refined Monte Carlo (r-MC) simulation (Davey, 2011). Importantly, published findings from *Fr* 13 assessments have generally underscored that current risk assessments actually downplay the real risks in bio-process failures and survival of unwanted micro-organisms (Cerf & Davey, 2001; Davey et al., 2011, 2012, 2013; Patil et al., 2005).

A seminal Fr 13 assessment of UV irradiation was presented by Davey et al. (2012) for Escherichia coli in the presence of suspended solids (as Celite 503TM with a mean particle size of 23  $\mu m$ , (Amos et al., 2001)) in a simplified, laminar flow reactor. They showed that some 47 in every 10,000 continuous UV operations could unexpectedly fail due to random effects in UV parameters. This was despite a tolerance of 10% in the design to reduce viable numbers of E. coli by  $10^{-4}$ . This meant high levels of survival of viable E. coli would occur each 0.58 years of continuous operation, that is, a failure on average each six calendar months in an otherwise apparently well-run and well-maintained operation. E. coli was chosen as the indicator micro-organism because it is a species of coliform bacteria specific to faecal material from humans and other warm-blooded animals and is a widely used indicator for health risk in potable water. A drawback was the simplified nature of the laminar flow model used.

#### 1.1. This study

Here a Fr 13 random assessment is presented for the first time of a more practical UV irradiation model with turbulent flow of water. It is based on the extensive experimental data of Ye (2007) and Ye. Forney, Koutchma, Giorges, and Pierson (2008). The aims were to demonstrate how random changes in UV parameters can contribute to unwanted and surprise failure of UV irradiation in an otherwise apparently well-operated and well-maintained series annularreactor, and; to determine the likely success of proposed intervention strategies to minimize risk of failure and improve safety. Operating conditions are chosen with a view to applying findings to realistic problems related to large-scale UV irradiation for potable water production. A unit-operations model is first developed and solved using a traditional single point assessment. This is then contrasted with results from the new Fr 13 assessment. A comparison is made of results with the earlier laminar flow model of Davey et al. (2012). The implications of Fr 13 assessments as a new quantitative tool to evaluate practical re-design and targeted physical changes to UV plant for improved safety is briefly discussed.

#### 2. Materials and methods

#### 2.1. The annular UV reactor of Ye (2007)

The configuration of the continuous flow UV reactor of Ye (2007) and Ye et al. (2008) is an annular thin film in a concentric cylinder. The annular geometry is used because it is suitable for inactivating micro-organisms in for example fruit juices. A schematic is shown as Fig. 1. As is seen a single UV lamp sits in the central axis of the reactor. Fluid flow is in the annular gap. Depending on flow rates, flow in this gap can be turbulent or laminar. Turbulent flow is used to increase UV efficacy (Severin, Rittmann, & Engelbrecht, 1984).

A unit-operations model of UV irradiation with turbulent flow in the annular-reactor can be developed as a plug flow reactor (PFR) (Levenspiel, 1999) in which first-order kinetics for UV inactivation of *E. coli* is assumed such that:

$$\ln\left(\frac{N}{N_0}\right) = -kI_{av}\tau\tag{1}$$

(All symbols used are defined in the Nomenclature). The bulk residence time of the water is:

$$\tau = L/\nu \tag{2}$$

The average (bulk) water velocity is obtained from:

$$v = \frac{Q}{\pi (R_2^2 - R_1^2)}$$
(3)

Assuming the flow is uniform (steady-state), the average fluence distribution is given by Ye (2007):

$$I_{av} = 2 \frac{\pi \int_{R_1}^{R_2} I_0 \frac{R_1}{r} \exp(-\alpha(r-R_1)) r dr}{2\pi \int_{R_2}^{R_1} r dr} = \frac{I_0 R_1 [1 - \exp(-\alpha(R_2 - R_1))]}{0.5\alpha \left(R_2^2 - R_1^2\right)}$$
(4)

Substituting for *I*<sub>av</sub> from Eq. (4) into Eq. (1) gives:



Fig. 1. Schematic diagram of a thin film annular-reactor between two concentric cylinders. Adapted from Ye, 2007.

(5)

$$\ln\left(\frac{N}{N_0}\right) = -k\frac{R_1[1 - \exp(-\alpha(R_2 - R_1))]}{0.5\alpha(R_2^2 - R_1^2)}I_0\tau$$

If  $\alpha$   $(R_2-R_1)>5$  and exp  $(-\alpha$   $(R_2-R_1)) <<$  1, Eq. (5) can be simplified to:

$$\ln\left(\frac{N}{N_0}\right) = -\frac{kl_0\tau R_c}{\alpha d} \tag{6}$$

where the gap is:

$$d = R_2 - R_1 \tag{7}$$

A new dimensionless group where radiation comes from the inner cylinder was defined by Ye (2007) as:

$$R_{\rm c} = \frac{2R_1}{R_2 + R_1} \tag{8}$$

A ratio  $(c/\delta)$  is used to correct Eq. (6) for deviations between a real reactor and the PFR such that:

$$\ln\left(\frac{N}{N_0}\right) = \frac{-ckI_0\tau R_c}{\alpha d\delta} \tag{9}$$

For base log<sub>10</sub> Eq. (9) is given as:

$$\log_{10}\left(\frac{N}{N_0}\right) = \ln\left(\frac{N}{N_0}\right) / 2.303 \tag{10}$$

The boundary layer thickness for turbulent flow  $(\delta)$  is:

$$\delta = \frac{2\mu}{\rho v f} \tag{11}$$

The dimensionless friction factor (f) is given by:

$$f = 0.079 \mathrm{Re}^{-0.25} \tag{12}$$

where the Reynolds number is:

#### $\mathrm{Re}=2d ho v/\mu$

Eq. (1) to Eq. (13) defines the unit-operations model for UV irradiation for potable water in turbulent flow in the annular-reactor. To obtain the required reduction in the number of viable *E. coli* 

contaminants a 4-series experimental annular-reactor was used by Ye (2007) and Ye et al. (2008). A schematic is shown in Fig. 2. Each annular-reactor consisted of a single, low-pressure, germicidal UV lamp (UltraDynamics model TF-1535, Severn Trent Services Inc., Colmar, PA) surrounded by a quartz inner-cylinder and stainless steel outer-cylinder. The total irradiated length was L = 196.2 cm with a total incident fluence for the 4-lamps of  $I_0 = 55.4$  mW cm<sup>-2</sup>. The radius of the quartz inner-cylinder was  $R_1 = 1.225$  cm and the radius of the steel outer-cylinder was  $R_2 = 1.74$  cm (giving a gap of 0.515 cm). A flow rate of Q = 180 mL s<sup>-1</sup> was used to promote turbulent flow (Re > 2100). The value of the first-order UV inactivation constant for *E. coli* in water was determined (Ye, 2007) as k = 0.325 mW<sup>-1</sup> s<sup>-1</sup> cm<sup>2</sup> and the value of the absorption coefficient for water from the data of Koutchma (2009) is  $\alpha = 0.01$  cm<sup>-1</sup>.

#### 2.2. Traditional single point simulation

Traditionally, for simulation of unit-operations in foods applications a single point, deterministic and expected value (that is, Single Value Assessment, SVA) with or without sensitivity analyses (Sinnott, 2005) is used (Davey, 2011; Davey et al., 2013). For the annular UV irradiation reactor this is done as follows: for the



Fig. 2. The 4-series annular-reactor of Ye. Adapted from Ye et al., 2008.

physical system defined by  $R_1$ ,  $R_2$ , L and Q, v = 37.5 cm s<sup>-1</sup> from Eq. (3). Substitution into Eq. (2) yields  $\tau = 5.3$  s. From, respectively, Eq. (7) and Eq. (8), d = 0.515 cm and  $R_c = 0.826$  (dimensionless). Additionally, with  $\mu = 0.93 \times 10^{-3}$  Pa·s (Ye, 2007) and, for water at 20 °C,  $\rho = 998.2$  kg m<sup>-3</sup> (Crittenden, Trussell, Hand, Howe, & Tchobanoglous, 2012), Eq. (13) yields R = 4148 (dimensionless). Substitution into Eq. (12) yields f = 0.0098 (dimensionless). Substitution f f, together with a value for the kinematic viscosity of water at 20 °C of  $v = 1.004 \times 10^{-6}$  m<sup>2</sup> s (Crittenden et al., 2012) into Eq. (11) gives  $\delta = 188.5$  cm.

Substitution of values for *c*, *k*, *l*<sub>0</sub>,  $\tau$ , *R*<sub>c</sub>,  $\alpha$ , *d* and  $\delta$  into Eq. (9) gives a reduction in the number of viable *E*. *coli* of ln *N*/*N*<sub>0</sub> = -10.02 (dimensionless). From Eq. (10) the value is  $\log_{10} N/N_0 = -4.35$  (dimensionless), which is the more widely used basis for expressing reductions in viable contaminants in treated waters.

#### 3. Fr 13 simulation

(13)

#### 3.1. Defining UV failure

A fundamental requirement in *Fr* 13 risk assessments is a practical and unambiguous definition of failure (Davey, 2011). For the annular-reactor this will be unexpected, high levels of survival of *E. coli* post UV treatment.

A process risk factor (p) can be defined mathematically in terms of the aimed for log<sub>10</sub> reduction in viable *E. coli* and the actual process reduction. For added safety, a process tolerance (%tolerance) can be used; the meaning of which is that the reactor should operate to give the minimum design reduction, plus an additional reduction, in viable *E. coli*. Mathematically p is therefore given by:

$$p = -\% \text{tolerance} + 100 \left| 1 - \frac{\log_{10} \left( \frac{\widehat{N}}{N_0} \right)}{\log_{10} \left( \frac{N}{N_0} \right)} \right|$$
(14)

where  $\log_{10}(\hat{N}/N_0)$  is an instantaneous value of  $\log_{10}(N/N_0)$ . This form is actually computationally convenient (Davey et al., 2013) because for all p > 0, UV irradiation fails.

#### 3.2. r-MC sampling

In Fr 13 simulation the key input parameters are not defined by a point value as with traditional SVA, but by a distribution of values and the probability of each that can actually occur in practical operation. The Fr 13 simulation output is therefore not a single value but a distribution of values with the probability of each event occurring (Davey, 2011; Davey et al., 2013). A refined Monte Carlo (r-MC) sampling is used to simulate the input parameter. This is because "pure" Monte Carlo cannot be relied on to replicate the parameter distribution as it can both over- and under-sample from various parts of the distribution (Davey, 2010; Davey et al., 2013; Vose, 2008). The refinement is Latin Hypercube sampling (Vose, 2008) which ensures that values are sampled from each probability distribution to cover the entire practical range. To ensure that the output conforms to a Normal distribution a minimum number of random samples are necessary (Vose, 2008). This is usually some 1000 to 50,000 samples (Davey, 2011; Davey et al., 2013) (this, in any event, can be checked readily by visual inspection of the output distribution).

## 3.3. Fr 13 model

Eq. (1) through Eq. (14), together with r-MC sampling of the defined probability distributions of input parameters, defines the Fr 13 unit-operations model for UV irradiation for potable water in turbulent flow in the annular-reactor. The Fr 13 model is therefore identical in form to the traditional model in that all mathematical operations (additions, multiplications, integrations etc.) that connect parameters are the same except that a probability distribution is used instead of a single value with error estimate (Davey, 2010, 2011; Davey et al., 2013; Sinnott, 2005).

Calculations to simulate turbulent flow in the annular-reactor were carried out using Microsoft Excel<sup>TM</sup> with a commercially available add-on @Risk<sup>TM</sup> (version 5.5, Palisade Corporation). An advantage of this is that Excel has nearly universal use and thereby makes communication of results streamlined. A practical process tolerance of plus 10% on the required log10 reduction of viable E. coli was assumed (Brigitte Carpentier, Laboratoire de securite sanitaire de Maisons-Alfort, France, pers. comm.).

#### 4. Results

Table 1 presents a summary comparison of results from the traditional SVA and the new Fr 13 simulation of UV irradiation of water in turbulent flow in the annular-reactor of Ye (2007) and Ye et al. (2008). Because the physical system has been fixed by: c, L,  $\alpha$ ,  $\mu$ ,  $\rho$ , v,  $R_1$  and  $R_2$ , the key UV operating parameters are:  $I_0$ , k and Q. These are defined in column 1 of the table. The traditional SVA calculation, outlined above, is read down column 2 where the reduction in viable  $E.\ coli$  of  $10^{-4.35}$  is shown.

The Fr 13 illustrative simulation is read down column 3 in which a normal distribution is assumed for UV operating parameters: RiskNormal (mean, stdey, RiskTruncate (minimum, maximum)). For UV fluence the distribution used in the absence of hard commercial data is  $I_0 =$ **RiskNormal** (55.4, 5.54, **RiskTruncate** (49.86, 60.94)) to give a mean = 55.4 mW cm<sup>-2</sup> with a stdev = 10%, and minimum = 49.86 and maximum = 60.94 mW cm<sup>-2</sup>. This is a practical way of stating that in operation the UV lamp does vary randomly in time but that any change will not move outside this range. To acknowledge a natural biological variability in sensitivity to UV of the viable *E. coli* cells it is assumed k =**RiskNormal** (0.325,

#### Table 1

Comparison of traditional single point (SVA) and Fr 13 risk assessments for turbulent flow in 4-series annular-react

Parameters	SVA <sup>a</sup>	Fr 13 <sup>b</sup>	
$I_0 ({\rm mW}{\rm cm}^{-2})$	55.4	50.4575	RiskNormal (55.4, 5.54,
			RiskTruncate (49.86, 60.94))
$k (\text{mW}^{-1} \text{ s}^{-1} \text{ cm}^2)$	0.325	0.3247	RiskNormal (0.325, 0.0325,
			RiskTruncate (0.2925, 0.3575))
$Q (mL s^{-1})$	180.0	183.1978	RiskNormal (180, 18,
			RiskTruncate (162, 198))
$v (cm s^{-1})$	37.5	38.1841	Eq. (3)
$\tau(s)$	5.3	5.1383	Eq. (2)
d (cm)	0.5150	0.5150	Eq. (7)
R <sub>c</sub> (dimensionless)	0.8263	0.8263	Eq. (8)
Re (dimensionless)	4148	4221.4055	Eq. (13)
f (dimensionless)	0.0098	0.0098	Eq. (12)
δ (cm)	188.5	189.3633	Eq. (11)
$\ln N/N_0$	-10.02	-8.9166	Eq. (9)
(dimensionless)			
$\log_{10} N/N_0$	-4.35	-3.87	Eq. (10)
(dimensionless)			
p (dimensionless)		0.9810	Eq. (14)

<sup>a</sup> Traditional single point, or, Single Value, Assessment.
<sup>b</sup> One only of 10,000 scenarios.

0.0325, RiskTruncate (0.2925, 0.3575)) (Amos et al., 2001). The influence of pump variation on flow of water is defined as Q = RiskNormal (180, 18, RiskTruncate (162, 198)). This flow variation of 10% is considered usual for standard controllers (B K O'Neill, School of Chemical Engineering, The University of Adelaide, pers. comm.).

Ten thousand (10,000) Latin Hypercube random samples (r-MC) of each input operating parameter distribution were used to ensure a normally-distributed simulation output. This means in practice that all possible combinations of process scenarios that could occur in the UV unit-operation will have been simulated.

Importantly, data shown in column 3 of Table 1 for Fr 13 simulation are for one only scenario of these 10,000. A total of 1604 failures were identified in the 10,000 scenarios, which is about 16%. These are summarised in Fig. 3. The failures are seen to the right of the figure with all p > 0 and are therefore readily identified.

#### 5. Discussion

#### 5.1. Fr 13 failures

To highlight how these failures actually arise in practice, 25 were randomly selected and are presented as Table 2. A practical



Fig. 3. Distribution for the risk factor (p) for UV irradiation for potable water in turbulent flow in the 4-series annular-reactor

Table 2	
Twenty (25) selected failures from	1604 in 10,000 UV irradiation scenarios.

Row	Volumetric flow Q (mL s <sup>-1</sup> )	Incidence fluence I <sub>0</sub> (mW cm <sup>-2</sup> )	Inactivation constant <i>k</i> (mW <sup>-1</sup> s <sup>-1</sup> cm <sup>2</sup> )	Risk factor p (dimensionless)
1	194.7383	52.0955	0.3432	0.0082
2	182.3258	54.0445	0.3037	0.2893
3	191.4998	53.6160	0.3243	0.6276
ª4	183.1978	50.4575	0.3247	0.9810
5	168.4671	50.0433	0.2942	1.1751
6	182.8244	52.5624	0.3097	1.3250
7	196.9552	52.5334	0.3389	1.6494
8	190.7225	52.0797	0.3270	2.0072
9	186.3105	52.8802	0.3114	2.4112
10	185.5021	51.1656	0.3188	2.7596
11	168.5156	50.3493	0.2948	0.4675
12	194.1587	50.0273	0.3435	3.1645
13	189.2170	55.0680	0.3007	3.6106
14	182.8628	52.8269	0.2983	4.1905
15	191.5682	54.8932	0.3025	4.6784
16	182.5216	51.7166	0.3002	5.2695
17	168.7240	50.1579	0.2958	0.6523
18	185.9576	52.1671	0.3025	5.8501
19	189.8552	54.4526	0.2954	6.4244
20	194.6565	50.4537	0.3266	7.0169
21	196.1355	56.1733	0.2927	7.9741
22	182.4156	50.6671	0.2927	8.9987
23	168.8120	50.0162	0.2986	0.1102
24	188.5492	49.9029	0.3032	10.6892
25	169.9687	51.0380	0.2927	0.8788

<sup>a</sup> Particular scenario of Table 1.

advantage of the data in this table is that the particular combination of UV parameters that resulted in the failure can be easily identified. An example in bold print (row 4 of the table), shows the particular combination of randomly sampled values for Q = 183.2 mL s<sup>-1</sup>,  $I_0 = 50.46$  mW cm<sup>-2</sup>, and; k = 0.3247 mW<sup>-1</sup> s<sup>-1</sup> cm<sup>2</sup>, resulted in greater survival of *E. coli* than designed and therefore failure to produce potable water. This is underscored by the corresponding value of the risk factor of p = 0.981 and, is the particular scenario presented in Table 1. It is interesting to note that for this combination Q is greater than the mean,  $I_0$  less than the mean and k very nearly equal to the mean, of the practical distributions used to define the parameters.

Other combinations of parameters can be readily identified in the table. For example, in row 25, Q is less than the mean, indicating a longer residence time of the water in the annular-reactor and therefore the chance for reduced survival of *E. coli*; but the corresponding values of UV fluence ( $I_0$ ) and inactivation constant (k) for viable *E. coli* are also less than the mean values of the distribution. This chance combination of process parameters results in UV failure (p = 0.8788). In summary, a detailed study of all 1604 combinations of the three UV process parameters that resulted in p > 0, underscores that the UV success or failure cannot be intuitively "guessed" directly from parameter values.

Clearly, the greater the number of process parameters in a unitoperation the more difficult it becomes to intuit success or failure of the operation based on a sound knowledge of the particular values of process parameters. This fact underscores the elegant utility of the risk factor, especially with increasing complexity in any unitoperation.

#### 5.2. Visualizing Fr 13 risk

Although the tabulated data of Table 2 do give a practical insight into UV operation, a difficulty is to gain an immediate overall perspective, or visualisation, of p values that actually underscore UV failure for potable water. To try to achieve this, a 3D plot of the 25 selected values from Table 2 was produced using commercially available software (Statistica<sup>TM</sup> version 10, StatSoft Inc.) and is presented as Fig. 4. Part a) of this figure shows a scatter plot for the three UV parameters, respectively, Q,  $I_0$  and k. The plot in part b) shows the surface plot for all 25 values p > 0. The random nature of the p values in time with continuous operation means that the surface plot cannot be extrapolated in any reliable way. It does serve to show however that at the values of Q greater than the mean (>180 cm L s<sup>-1</sup>) UV is increasingly likely to fail with the unwanted survival of viable *E. coli*. Whilst this graphical treatment seems to work for the three parameter unit-operation model for this study, a radar plot could be more useful with increased numbers of key parameters in increasingly sophisticated process models (Davey, unpublished data).

Importantly, the new *Fr* 13 risk simulation reveals that, on average, viable *E. coli* will unexpectedly survive UV treatment in greater number in the series annular-reactor in about 16% of all continuous operations over the long term, that is, 1604 in each 10,000 due to random effects within the physical system of the unit-operation. This will be despite apparent best operation and maintenance. If each simulation is considered an operating day, with prolonged periods of operation, this is translated as 1.92 ( $=1604/10,000 \times 12$ ) surprise (unexpected) failures each calendar month. However, it cannot be assumed these will actually be spaced evenly in time. Importantly this new insight is not provided



Fig. 4. Plot of the 25 selected Fr 13 failures (p > 0) of Table 2: 3D scatter plot (a) and 3D surface plot (b).

by alternative current risk methodology, with or without sensitivity analyses.

A Fr 13 simulation can be thought of as an extended risk sensitivity analysis of how often the UV could probably failed. This is because all combinations of parameters that could actually occur in practical operations are considered and quantified.

#### 5.3. Input probability distributions for Fr 13

An important consideration that arises with the carrying out any *Fr* 13 risk assessment is how the value of the risk factor (*p*), and therefore the predicted surprise failure frequency, will be impacted by the probability distribution used to define the key operating parameters. Clearly, the more realistic the input probability distribution used for key parameters, the better the simulation for *Fr* 13 failure. In general, the most realistic simulations will made with hard data, or expert knowledge. These aspects have been discussed earlier (Davey, 2010; Davey et al., 2013); to summarize, there are in principal some 40 distribution types (Vose, 2008) that might be used, including: *Triangle, Beta Subjective, Tnormal* (e.g. Cerf & Davey, 2011; Davey & Cerf, 2003) and *Normal* (Davey, 2011; Davey et al., 2013; Patil et al., 2005), all with or without truncations (Davey, 2011):

Truncation is an important characteristic. From a practical point of view for example, were a *Normal* probability distribution used, for say, atmospheric pressure (mmHg) the probability of atmospheric pressure being near zero, or 1000 (mmHg) in any fixed global location is small. Rather, there will be a practical range that simulates the experienced atmospheric pressures over a long period, so the distribution must be realistically truncated to reflect this, say 720 (minimum) to 790 (maximum), mmHg.

In this study, in the absence of alternate data, the 1 stdev assumed about the mean with the **RiskNormal** distributions for all three key UV parameters,  $l_0$ , k and Q, means that 2/3 (68.2%) of all r-MC values sampled will fall in this interval (Sullivan, 2004). The distributions used have also been truncated (*minimum* = mean - 1 stdev) maximum = mean + 1 stdev) to approximate the most practical set of realistic values and outcomes for p.

With the **RiskNormal** distribution, a 3 stdev will mean nearly all r-MC samples (99.7%) will fall in this interval (Sullivan, 2004). Repeat simulations were carried to test the impact of an increased variance of 3 stdev about the **RiskNormal** mean and **RiskTruncate** (minimum and maximum) in each of the three key parameters,  $I_0$ , k and Q of the *Fr* 13 unit-operations model for UV irradiation for potable water. For example for  $I_0$ , the input probability distribution becomes **RiskNormal** (55.4, 16.62, **RiskTruncate** (38.78, 72.02)). Results show that the impact is to give a failure rate of 13%. This is not considered meaningfully different from that of 16% (1 stdev).

Some experimenting will generally show that the failure frequency is not highly sensitive to a range of distributions (Davey, unpublished data). A Normal distribution is however readily justified in the absence of contrary hard data or theoretical considerations.

The overriding criterion in selection of the probability distribution however is that each scenario outcome produced must be practically observable in real operation; the chance (probability) of each actually occurring is taken-care of in the distribution.

#### 5.4. Minimizing Fr 13 risk

Because Fr 13 surprise failure is due solely to random (chance) effects, more study or measurement cannot be used to reduce this type of vulnerability of the unit-operation. However, this situation actually leads to a very practical application of the Fr 13 method for improving design and safety. This is simulation in second-tier

studies (Davey, 2010, 2011; Davey et al., 2013) where Fr 13 failure can be minimized through proposed physical re-designs of the operation or through changes to variance in the key input parameters. This is illustrated in what follows.

For the annular UV irradiation reactor three options for improved safety and reduced vulnerability to *Fr* 13 risk are apparent. The first is to specify an increase in the safety tolerance. Repeat simulations are summarized in Fig. 5 for a range from 5 % to 30 %. It is seen that the number of *Fr* 13 failures, expectedly, falls away with increased tolerance and rises sharply with reduced tolerance. There is an apparent exponential dependence on failure rate with tolerance. The figure shows however the practical limit is about 30% after which no reduction in the number of *Fr* 13 failures is obtained.

A second is to reduce the variance on the continuous flow rate of water through the reactor (Q). In practice this means a muchimproved flow controller. Repeat simulations are presented in Fig. 6 for a range of values of the parameter distribution with a stdev of 2, 5, 8 and 10%. As expected the number of failure is seen to rise with increased stdev and fall away as stdev is decreased. This suggests that increased costs for improved process control with small fluctuations (low stdev) in water flows might be readily iustified.

A third is to reduce any variance on UV fluence ( $I_0$ ), that is, to improve the quality of the UV lamp. UV lamps do age with time (Bolton & Cotton, 2008). Repeat simulations show that a halving of the variance on fluence will reduce vulnerability of *Fr* 13 failures from 1604 to 1370. The cost of the UV lamp may increase significantly to achieve this.

Significantly however, from a practical view, it is not possible to reduce the susceptibility to UV irradiation of *E. coli* because of natural microbiological variability, and therefore no changes to the inactivation constant (k) can be purposely made in a physical redesign of the unit-operation.

#### 5.5. Turbulent vs laminar flow Fr 13 failures

A comparison can be made of results for the turbulent flow annular-reactor of Ye (2007) with those of the laminar flow reactor of Davey et al. (2012). A comparative summary is given as Table 3.

**Model I** shown in the table is the laminar-flow UV model (Davey et al., 2012) and **Model II** is the turbulent flow model of Ye



Fig. 5. Effect of %tolerance on log<sub>10</sub> reduction in viable *E coli* against the number of *Fr* 13 failures per 10.000 scenarios of continuous UV irradiation for potable water in the 4-series annular-reactor.



Fig. 6. Effect of variability (%-stdev) on the volumetric flow rate (Q = 180 mL s<sup>-1</sup>) against the number of Fr 13 failures in UV irradiation for potable water in the 4-series annular-reactor.

(2007) and Ye et al. (2008) used in the present study. Both models achieve the same design reduction in viable *E. coli* of  $-10^{-4}$ . An apparent contrast is the greater vulnerability to *Fr* 13 failure in continuous operation of 16% with **Model II** compared to 0.4% for **Model I**.

However, caution is needed as it is difficult to actually compare directly the difference between the two models since both have different parameters, for example **Model I** includes UV-shielding suspended solids while **Model II** includes absorption coefficient. However, overall it is satisfying that the first-order inactivation kinetics for both is similar (for **Model I** is k = 0.4139 mW<sup>-1</sup>s<sup>-1</sup> cm<sup>2</sup> and k = 0.325 mW<sup>-1</sup>s<sup>-1</sup> cm<sup>2</sup> for **Model II**).

Because a relatively high flow rate is required to sustain turbulent flow with **Model II**, a 4-series reactor was necessary to give the needed residence time ( $\tau = 5.22 \text{ s}$ ). Useful further direct contrast is limited because the two assessments involve different defined parameter distributions ( $I_0$ , Q and k for **Model II**;  $I_0$ ,  $\tau$  and concentration of UV-shielding material for **Model II** could now be extended to include effects of both UV-shielding and UV-absorbing suspended solids using, for example, the published experimental data of Amos et al. (2001). The concentrations for both these effects on UV could be defined to usefully and more realistically simulate water quality and flows and fluctuations for particular geographical sites or industries.

#### Table 3

Comparison of Model I (laminar flow reactor of Davey et al. (2012)) with Model II (turbulent flow annular-reactor of Ye (2007) and Ye et al. (2008)) for UV irradiation of *E*. coil for potable water.

Parameter	Model I (simplified laminar flow)	Model II (4-series annular-reactor)
Reactor flow regime	Laminar	Turbulent
Fluence, $I_0$ (mW cm <sup>2</sup> )	11.9	55.4
Residence time, $\tau$ (s)	1.90	5.22
First-order UV inactivation constant, k (mW <sup>-1</sup> s <sup>-1</sup> cm <sup>2</sup> )	0.414	0.325
$\log_{10}(N/N_0)$ , (dimensionless)	-4.08	-4.35
Fr 13 failures, (%)	0.4	16
Description	Too simplified (?), but includes suspended solids	Sophisticated analysis, involves absorption properties, no suspended solids

Other contaminant water micro-organisms could also be incorporated, especially *Giardia* (Linden, Shin, Faubert, Cairns, & Sobsey, 2002). *Giardia* is a prevalent and relatively resistant water pollutant that can be treated with UV irradiation (Gibson, Haas, & Rose, 1999; Linden et al., 2002).

#### 5.6. Coupling Fr 13 with commercial technologies

The valuable insight to be gained with *Fr* 13 risk modelling over traditional methods is to quantitatively identify all process scenarios that are probable, including surprise failures.

The fact that the Fr 13 risk modelling is predicated on universal unit-operations principles has led to hypotheses that it could be coupled with commercial technologies, such as Aspen Plus<sup>®</sup> or Batch Process Developer<sup>®</sup>, to produce significantly more powerful process design and assessment tools than are currently available (Davey, 2010).

#### 6. Conclusions

A new Fr 13 risk analysis of turbulent flow UV irradiation for potable water in the annular-reactor of Ye (2007) and Ye et al. (2008) has highlighted that failure, defined by unexpected survival of viable *E. coli* post-treatment, can result from random effects in prolonged continuous operation.

The number of failures is related to the combined effects of variance about process parameter mean values. This means that continuous operation is actually a mix of successful and failed states, and neither "human error" nor "faulty fittings" (Davey, 2011) need to be invoked as an explanation. Importantly these *Fr* 13 insights are not available from current risk analyses. Reducing the variance in key parameters, through for example improved process control, whilst potentially costly, can minimize likelihood of UV failures.

Fr 13 failure assessments can be used in second-tier studies to quantitatively assess risk from proposed changes in control or design and intervention strategies, and therefore can be used to guide improvements to better process safety and equipment.

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#### Nomenclature

	constant to correct for deviation between a real and idea
	PFR reactor, cm
1	annular gap width, cm
	friction factor, dimensionless
av	average fluence of ideal plug flow reactor, mW cm <sup>1</sup>
0	incident fluence, mW cm <sup>2</sup>
c	inactivation constant, mW <sup>1</sup> s <sup>1</sup> cm <sup>2</sup>
	length of radiation section, cm
V	concentration viable Escherichia coli, CFU mL <sup>1</sup>
V <sub>0</sub>	concentration viable E. coli before UV exposure, CFU mL
,	risk factor, dimensionless
PFR	plug flow reactor
2	volumetric flow rate, mL s <sup>-1</sup>
R1	radius of inner cylinder, cm
R2	radius of outer cylinder, cm
Rc	dimensionless group

- Re Reynolds number, dimensionless
- stdev standard deviation
- average water velocity in annular gap, cm s<sup>-1</sup> v

Greek symbols

- absorption coefficient, cm 1 α
- â boundary layer thickness, cm
- dynamic viscosity of water, 0.93  $\times$  10  $^{-3}$  Pa  $\cdot s$ μ
- density of water at 20 °C, 998.207 kg m p
- τ average residence time, s
- kinematic viscosity of water at 20 °C, 1.004  $\times$  10  $^{-6}$  m  $^2$  s u

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## Friday 13th Risk Modelling: A New Risk Model of UV Irradiation for Potable Water

*IAFP 2013*, Marseille, France, May 15-17. <u>http://www.foodprotection.org/europeansymposium/2013/</u>



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## Friday 13th Risk Modelling: A New Risk Model of UV Irradiation for Potable Water

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**Introduction**: Ultraviolet (UV) irradiation for potable water is an alternative to widespread disinfection methods using chlorine. However, sudden and unexpected failure of UV irradiation can lead to enduring public health effects, with or without fatalities. Here a new risk analysis of UV irradiation for potable water is presented using *Friday 13<sup>th</sup>* risk modelling (*Fr 13*) and a comparison made with current risk methods.

**Purpose**: The aim was to gain an understanding of possible effects of stochastic (random) changes in plant parameters on plant behaviour. Failure is defined as unexpected survival of pathogenic *Escherichia coli*.

**Methods**: The analysis is based on a unit-operations model and experimental data derived from Ye (2007). A failure factor (*p*) is defined in terms of a design reduction and actual reduction in viable *E. coli* as affected by stochastic change. UV irradiation is simulated using a refined Monte Carlo sampling of plant parameters.

**Results**: Results show that with an overtreatment tolerance of 15 % on the design reduction some 2.8 % of all UV operations can unexpectedly fail. This translates, on average, to a failure nearly each month of continuous operation. This insight is not available from current risk methods, with or without sensitivity analyses.

**Significance**: The *Fr 13* analysis is a significant advance on current risk methods because it produces all possible practical UV operations and outcomes. This quantitative insight can be used to assess re-design and targeted physical changes to UV plant for improved safety in operation.

## Impact of Suspended Solids on *Fr 13* Failure of UV Irradiation for Inactivation of *Escherichia coli* in Potable Water Production with Turbulent Flow in an Annular Reactor

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## Impact of suspended solids on *Fr* 13 failure of UV irradiation for inactivation of *Escherichia coli* in potable water production with turbulent flow in an annular reactor

## CrossMark

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#### HIGHLIGHTS

#### UV efficacy for potable water significantly impacted by initial suspended solids.

- However UV efficacy not vulnerable to fluctuations in suspended solids.
- Overall UV efficacy is a mix of successful and unsuccessful inactivation of *E. coli*.
- Results can be used to improve UV efficacy, reliability and safety.
  Benefit to designers, operators and
- Benefit to designers, operators and risk analysts of UV treatment for potable water.

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G R A P H I C A L A B S T R A C T

Distribution of risk factor (p) of UV irradiation of visble E. co

#### ABSTRACT

Ultraviolet irradiation (UV) is an important alternative to disinfection for production of potable water. Viable Escherichia coli is a widely used indicator for public health risk. However, UV efficacy is reduced by suspended solids that can act as both UV shielding and UV absorbing, agents. Failure of UV irradiation can lead to an enduring health legacy. Here the probabilistic *Fr* 13 methodology of Davey et al. (2015) is demonstrated for turbulent flow of feed water with suspended solids irradiated in an annular reactor and, a comparison made with the traditional deterministic method. The aim was to examine the impact of naturally occurring fluctuations in suspended solids concentration on failure to inactivate viable E. coli. A UV failure factor (p) is defined in terms of the design and actual log<sub>10</sub> reduction in viable *E. coli.* UV irradiation is simulated using (Latin Hypercube) Monte Carlo sampling. Illustrative overall results show some 32.1% and 43.7% of apparent successful operations could unexpectedly fail over the long term due, respectively, to combined impact of random fluctuations in feed water flow (Q), lamp intensity ( $I_0$ ) and shielding and absorption of UV by suspended solids [conc]. This translates to four (4) failures each calendar month (the comparison rate without suspended solids is 16% or two (2) failures per month). An unexpected finding however is, although the initial presence of sus-pended solids as both UV shielding (median particle size 23 µm) and absorbing agent has a highly significant impact on reducing UV efficacy, fluctuations in concentration of these in the feed water do not meaningfully impact overall vulnerability. UV failure is impacted highly significantly by fluctuation in feed water flow. It is concluded this is strong quantitative evidence to emphasize that solids should be removed prior to the UV reactor, and that an improved flow control be used to reduce variance on feed water flow, rather than increased UV dose. This work will be of benefit to operators of UV equipment and researchers in risk analyses. Crown Copyright © 2015 Published by Elsevier Ltd. All rights reserved.

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#### 1. Introduction

Ultraviolet irradiation (UV) is a practical alternative to halogen disinfection e.g. chlorine for production of potable water (Bitton, 2011; Amos et al., 2001; Das, 2001). The post-treatment presence of viable *Escherichia coli*, a pathogenic contaminant, is widely used as an indicator of efficacy of potable water production and health risk (Stevens et al., 2003; Loge et al., 1999). Failure of UV irradiation to reduce these viable pathogens to a safe level can lead to an enduring public health legacy.

A reliable and quantitative understanding of risk of UV irradiation for potable water is therefore important.

An emerging risk methodology is that of Davey and co-workers. Their thesis is that naturally occurring, chance fluctuations in otherwise well-operated plant parameters can accumulate in onedirection and lead unexpectedly to surprise (sudden) failure in either process or product about a binary divide. They called this Fr 13 (Friday 13th) failure to underscore the nature of the occurrence. Published studies include surprise failure of a large-scale, coalfired-boiler from thermally efficient to inefficient (Davey, 2015), pasteurization failure of raw milk to meet regulatory standards (Chandrakash et al., 2015), failure of Clean-In-Place from successful removal of whey protein deposits to failure to remove these (Davey et al., 2015; 2013; Chandrakash, 2012), failure in continuous UV irradiation from potable to non-potable water (Abdul-Halim and Davey, 2015; Davey et al., 2012), from stable fermentation to un-stable (washout) (Patil, 2006; Patil et al., 2005), failure of batch-continuous UHT milk from sterile to non-sterile (Davey and Cerf, 2003; Cerf and Davey, 2001), and; more generally, from safe to unsafe operation (Davey, 2011; Nolan and Barton, 1987). Overall, this work shows that without breakage, shutdown or faulty fittings, well-operated and well-maintained continuous operations can in fact be an instantaneous mix of successful and failed operations (Davey, 2015; Gujer, 2008).

A practical advantage claimed for *Fr* 13 is that all process scenarios that could exist can be quantified, including failures. It is claimed to be more mathematically correct than alternate risk and hazard methods because knowledge about the process is separated from impact of random fluctuation in parameters (Abdul-Halim and Davey, 2015; Davey et al., 2015; Rai and Krewski, 1998; Hoffman and Hammonds, 1994). It therefore has the advantage that it permits the effect of each to be studied (Davey, 2015).

The possible risk with fluctuation in parameters about a steadyvalue is the focus of recent approaches of Aven (2010) and Haimes (2009), and Milazzo and Aven (2012). A key drawback however is that these approaches remain largely qualitative, and are not rigorously quantitative.

Importantly, Fr 13 is based on established unit-operations (Foust et al., 1980; Wankat, 2007; McCabe et al., 2001) and not subjective or qualitative views of 'credible' risk scenarios as with this approach, and others, for example, HAZOP and HACCP.

As highlighted in the Blackett review (Anon, 2012) low probability, high impact failures are a major theoretical and practical concern for companies and governments of almost every size. In potable water production these failures are acknowledged as real events and can have a significant 'snow-ball' effect in determining the end quality of integrated processes. Remarkably, *Fr 13* event is a notion that has long persisted in the industrial West (Suddath, 2009).

An initial Fr 13 assessment of UV irradiation was presented by Davey et al. (2012) for a simplified, laminar flow reactor with E. coli as contaminant. Results revealed that 0.4% of UV operations over the long term could unexpectedly fail due to the accumulated impact of naturally occurring random fluctuations in UV intensity and residence (treatment) time. A drawback however was the simplified nature of the laminar model used. To overcome this, an improved UV irradiation model was synthesised by Abdul-Halim and Davey (2015) for more usual turbulent flow in an annular reactor based on the work of Ye (2007). Results showed 16% of apparent successful operations, over the long term, could fail to achieve the Regulatory (Anon, 2013; Sommer et al., 2008) design reduction in viable *E. coli*  $\geq 10^{-4}$  due to the impact of random effects.

It is widely known however that UV efficacy is reduced by the presence of suspended solids as these can both absorb UV light and shield contaminants from UV (Cantwell and Hofmann, 2011; Winward et al., 2008; Amos et al., 2001; Emerick et al., 2000; Loge et al., 1999; Parker and Darby, 1995). There is a need therefore for a quantitative risk assessment of the impact of suspended solids on UV irradiation efficacy and possible UV failure for potable water production with turbulent flow.

#### 1.1. Purpose of this study

Here, we extend the work of Abdul-Halim and Davey (2015) to quantitatively assess the impact of naturally occurring random fluctuations in concentration of suspended solids on vulnerability to *Fr* 13 failure of UV irradiation for potable water production. *E. coli* is used as the indicator pathogen. The aim was to quantitatively investigate the impact of accumulated naturally occurring chance fluctuations in the concentration of suspended solids, together with those in UV lamp intensity and feed water flow on inactivation of *E. coli*.

A unit-operations model incorporating suspended solids, as both shielding and absorbing agents, on UV inactivation of *E. coli* based on published work is synthesised and solved using traditional, deterministic methods. Findings are contrasted with the new *Fr* 13 methodology. Results are compared with previous findings and used to assess practical re-design to minimize vulnerability to *Fr* 13 failure of UV irradiation of water with suspended solids present.

A justification for this work is that incorporation of, and knowledge about, the impact of suspended solids will lead to improved and more realistic simulations and therefore improved UV designs, reliability and safety.

#### 2. Materials and methods

#### 2.1. UV inactivation of E.coli with suspended solids present

Amos et al. (2001) presented extensive experimental data (n=40) and analyses for UV inactivation of E. coli ATCC 25922 (FDA strain, Seattle 1946) in the presence of suspended solids, and the development and assessment of four predictive model forms. Experimental work was carried out in a commercial UV Unit (Model LC-5, Ultraviolet Technology Australasia Pty Ltd., Australia). The suspended solids used to alter the (reverse osmosis) water transmittance were diatomaceous earth (as Celite 503™) for controlled UV shielding (89% SiO2 with median particle size 23 µm), and coffee powder (International Roast™) for controlled UV absorbing. Model forms evaluated included classical log-linear, Davey linear-Arrhenius (DL-A) (Ross and Dalgaard, 2004; McMeekin et al., 1993; Davey, 1993), square-root (i.e. Ratkowsky-Belehradek) (Ratkowsky, 1990; Belehradek, 1926) and a thirdorder polynomial (nOP). Test criteria for model rankings were based on the goodness of fit (percent variance accounted for (%V)) (Snedecor and Cochran, 1989), relative complexity (i.e. parsimony) (McMeekin et al., 1993; Davey, 1993), ease of synthesis and use, and; potential for physiological interpretation of coefficients.

The DL-A was found to best explain the data (%V=97.2) and overall best fulfilled the test criteria for a predictive model for

(2)

inactivation with both UV shielding and UV absorbing from suspended solids. The model form is given by

$\ln k = C_0 + C_1 \left[ dose \right] + C_2 \left[ dose \right]^2 + C_3 \left[ conc \right]$	(1)
where UV dose is	

and  $k=\mu W^{-1} s^{-1} cm^2$ . All symbols used are carefully defined in *Nomenclature*. The model is applicable to a range of concentration of shielding agent  $0.01 \le [conc] \le 0.3 \text{ g L}^{-1}$  and absorbing agent  $0.001 \le [conc] \le 0.03 \text{ g L}^{-1}$ .

The model form is said to be linear-Arrhenius and 'additive' (Ross and Dalgaard, 2004; Davey, 1993; Amos et al., 2001). The values for the model coefficients ( $C_0 - C_3$ ) are presented in Table 1 for UV inactivation of viable *E. coli* in the presence of both UV shielding and UV absorbing agents.

#### 2.2. An annular UV reactor unit-operations with turbulent flow

The unit-operations annular reactor of Abdul-Halim and Davey (2015) was based on the experimental work of Ye (2007) who used a single, low-pressure UV lamp surrounded by a quartz inner-cylinder and stainless steel outer-cylinder. The quartz inner-cylinder radius was  $R_1$ =1.225 cm and the steel outer-cylinder radius  $R_2$ =1.74 cm (creating a gap, d=0.515 cm). The irradiated (4-series) length was L=196.2 cm. For turbulent flow (Re > 2100), the water flow rate is Q > 180 mL s<sup>-1</sup>.

The unit-operations model presented by Abdul-Halim and Davey (2015) for turbulent flow in the annular-reactor was a plug-flow reactor (PFR) such that

$$\ln\left(\frac{N}{N_0}\right) = -\frac{ckl_0\pi R_c}{\alpha d\delta} \tag{3}$$

For a more convenient log<sub>10</sub> base, Eq. (3) was written

$$\log_{10}\left(\frac{N}{N_0}\right) = \ln\left(\frac{N}{N_0}\right)/2.303\tag{4}$$

The residence time of the water in the reactor was given by  $\tau = L/\nu$  (5)

The water velocity in the gap is

$$v = \frac{Q}{\pi \left(R_2^2 - R_1^2\right)}$$
(6)

A dimensionless group for radiation from the inner cylinder defined by Ye  $\left(2007\right)$  is

$$R_c = \frac{2R_1}{R_2 + R_1}$$
(7)

The annular gap dimension is

 $d=R_2-R_1$ 

 $[dose] = I_0 \tau$ 

The ratio ( $c/\delta$ ) was used by Ye (2007) to correct for deviation of a real reactor from a PFR.

The boundary layer for turbulent flow ( $\delta$ ) is

$$\delta = \frac{2\mu}{\rho o f}$$
(9)  
The friction factor (f) is  
 $f = 0.079 \text{Re}^{-0.25}$ 
(10)  
where

$$Re = 2d\rho v/\mu \tag{11}$$

in which 2*d* is the hydraulic diameter for the annulus (outer–inner, cylinder diameter). The transition from laminar to turbulent flow

occurs when  $2000 \le Re \le 4000$  and a fully developed turbulent flow when  $Re \ge 4000$  (Koutchma et al., 2009).

Eqs. (1)–(11) defines UV irradiation for inactivation of viable *E. coli* for potable water in the presence of suspended solids in turbulent flow in the annular reactor of Ye (2007). For Eq. (3), c=0.0125 cm (Ye, 2007).

Importantly, Eqs. (3) and (4), show predicted log reductions in *E. coli* decrease with an increase in  $\alpha$  in this reactor. This is because influence decreased exponentially with path length from the UV radiation source i.e. 'small increases in  $\alpha$  resulted in large increases in under-irradiated volumes' (Ye, 2007). This was successfully experimentally demonstrated by Ye (2007) for this reactor (who concluded that a thin (much less than the d=0.515 cm) gap would need to be used for juices which have high values of  $\alpha$ ).

A value of the absorption coefficient  $\alpha$ =0.01 cm<sup>-1</sup> was used for UV treatment of the clean water of Abdul-Halim and Davey (2015), here however for contaminated water with suspended solids, this is assumed to be  $\alpha$ =0.0055 cm<sup>-1</sup> (Vasiliev and Alameh, 2008).

#### 2.3. Traditional single value assessment (SVA) simulation

Typically, in the water and food industries, unit-operations models are solved using a traditional, deterministic single point value, or single value assessment (SVA). This can be done with or without sensitivity analyses (Sinnott, 2005).

For the turbulent flow annular UV reactor defined by  $I_0 = 55,400 \ \mu\text{W cm}^{-2}$ ,  $Q = 500 \ \text{mL s}^{-1}$ ,  $L = 196.2 \ \text{cm}$ ,  $R_1 = 1.225 \ \text{cm}$ and  $R_2 = 1.74$  cm, and for the inactivation of viable *E. coli* defined by the model coefficients for UV shielding of Table 1, this is carried out as follows: from Eq. (6) v = 104.22 cm s<sup>-1</sup>;  $\tau = 1.9$  s from Eq. (5), and;  $[dose] = 104,298 \ \mu\text{W} \ \text{s} \ \text{cm}^{-2} \ \text{from Eq. (2)}. \ \text{From Eq. (1)} \ \text{(Table 1) at a} \ \text{mid-range} \ \text{value} \ [conc] = 0.115 \ \text{g} \ \text{L}^{-1}, \ k = 0.00136 \ \mu\text{W}^{-1} \ \text{s}^{-1} \ \text{cm}^2.$ Eqs. (7) and (8) respectively yield  $R_c = 0.8263$  (dimensionless) and d=0.515 cm. Given  $\mu=0.93 \times 10^{-3}$  kg m<sup>-1</sup> s<sup>-1</sup> (Ye, 2007) and, for water (20 °C)  $\rho$ =998.2 kg m<sup>-3</sup> (Crittenden et al., 2012), Eq. (11) yields Re=11,521 (dimensionless). From Eq. (10) f=0.0076 (dimensionless). The value of the kinematic viscosity of water (20 °C) used is  $v = 1.004 \times 10^{-6} \text{ m}^2 \text{ s}^{-1}$  (Crittenden et al., 2012). Substitution together with the value for f into Eq. (9) gives  $\delta = 243.39$  cm. The reduction in the number of viable E. coli is computed from substitution of values for c, k,  $I_0$ ,  $\tau$ ,  $R_0$ ,  $\alpha$ , d and  $\delta$  into Eq. (3) to give  $\ln N/2$  $N_0 = -2.13$  (dimensionless). From Eq. (4) therefore  $\log_{10}N/N_0 = -0.92$ (dimensionless).

Based on these experimental data of Amos et al. (2001) this is notably a highly significant reduction in UV efficacy in the annular reactor from the  $log_{10}$ =4.35 reported by Abdul-Halim and Davey (2015) due to the presence of UV shielding agent.

Similarly, for the presence of UV absorbing solids it can be shown,  $\log_{10}N/N_0 = -0.99$ .

#### 2.4. Fr 13 model and simulation

(8)

Failure of UV was defined by Abdul-Halim and Davey (2015) using a convenient dimensionless coefficient given by

$$p = -\% tolerance + 100 \left[ 1 - \frac{\log_{10}\left(\frac{\hat{N}}{N_0}\right)}{\log_{10}\left(\frac{N}{N_0}\right)} \right]$$
(12)

where  $\log_{10} \left(\frac{N}{N_0}\right)$  is an instantaneous value of  $\log_{10} \left(\frac{N}{N_0}\right)$  (or more mathematically correct, one possible scenario).

Eq. (12) is convenient because for all p > 0, UV irradiation will have failed. A practical process tolerance (margin) of plus 10% on the required  $\log_{10}$  reduction of viable *E. coli* was assumed by Abdul-Halim and Davey (2015) i.e. if the design  $\log_{10}$  reduction in

Table 2

Table 1 Coefficients for the Davey linear-Arthenius (DL-A) model for UV irradiation inactivation of viable *E*. *coli* in the presence of suspended solids as both UV shielding and UV absorbing agents  $\ln k = C_0 + C_1 [dose] + C_2 [dose]^2 + C_2 [conc]$  with *k* in  $\mu W^{-1} s^{-1} cm^2$  for a range of concentration of shielding agent  $0.01 \le [conc] \le 0.3 \text{ gL}^{-1}$ .

UV agent	C <sub>0</sub>	$C_1 \times 10^{-4}$	$C_2 \times 10^{-9}$	C3
Shielding	-6.344	-0.771	0.723	-0.685
Absorbing	-5.866	-1.14	1.30	- 11.04

viable *E. coli* plus 10% is not achieved, the UV treatment was said to have failed.

The *Fr* 13 failure model for UV irradiation of viable *E. coli* for potable water production with turbulent flow in the presence of suspended solids in an annular reactor is given by Eqs. (1)–(12).

In Fr 13 simulations, the key parameters are defined by probability distributions and not by single, 'best guess' values. These probability distributions are used to imitate the naturally occurring fluctuations in parameter values in time (Davey et al., 2015; Davey, 2011; Tucker et al., 2003; Vose, 1998). In the absence of unconditional (hard) data, normal distributions, which are truncated so as to obviate nonsensical values of the key parameters, have been used (e.g. Davey, 2015; Davey et al., 2015; Chandrakash, 2012; Davey, 2011; Patil, 2006; Patil et al., 2005). However, other types of distributions might be more suited if there are conditional data. For example, Davey and Cerf (2003) used a BetaSubjective distribution (Vose, 2008) to imitate residence time in a UHT milk plant, and a Triangle distribution (Vose, 2008) to imitate the decimal reduction time of viable populations of Bacillus stearothermophilus and Bacillus thermodurans. There are some 40 distribution types (Vose, 1998).

A refined Monte Carlo with a Latin Hypercube sampling (r-MC) is used to ensure values are sampled that cover the entire range of the distribution. (Sampling with 'pure' MC for e.g. cannot be relied on to replicate the distribution because it can both over- and under-sample from various parts of the distribution). If the number of samples is sufficiently large, the output mean of a product of a large number of independent positive parameters that have different distribution functions will be approximately normally distributed (Vose, 2008). Davey and co-workers (e.g. Abdul-Halim and Davey, 2015; Davey et al., 2015; 2013; Davey, 2011) have reported that this is usually some 1000-50,000 samples for typical unit-operations simulations. (The number is readily established when a plot of number of failures, all p > 0, versus number of r-MC samples has plateaued to a constant value). Importantly with a sufficiently large number of r-MC samples, all possible combinations of input parameter values and resulting output process scenarios that could occur in practical UV irradiations with suspended solids present will have been simulated, including failures.

The Fr 13 model is seen therefore to be identical to the traditional one in which all mathematical operations, additions, multiplications etc., that join parameters are the same, but one in which parameters are defined by distributions of values and not by single values (with error estimate); clearly therefore the Fr 13 output will be a distribution.

Simulations were carried out using Microsoft Excel<sup>TM</sup> with commercially available add-on @Risk<sup>TM</sup> (version 5.5, Palisade Corporation). Excel spread sheeting is advantageous as it has nearly universal use making communication of results straightforward. Additionally, the distributions defining naturally occurring fluctuations in parameters can be entered, viewed, copied and pasted and manipulated as Excel formulae. Ten thousand (10,000) samples were found sufficient.

Parameter	<b>SVA</b> <sup>a</sup>	Fr 13 <sup>b</sup>	
$I_0 (\mu W \text{ cm}^2)$	55,400	54046°	RiskNormal (55400, 1108),
			RiskTruncate (53184, 57616)
[conc] (g L <sup>1</sup> )	0.115	0.115°	RiskNormal (0.115, 0.0023),
			RiskTruncate (0.1104, 0.1196)
$O(mLs^{-1})$	500	495.84°	RiskNormal (500, 10), Risk-
			Truncate (480, 520)
L(cm)	196.2	196.2	Constant
$R_1$ (cm)	1.225	1.225	Constant
$R_2$ (cm)	1.74	1.74	Constant
$\mu$ (kg m <sup>-1</sup> s <sup>-1</sup> )	0.000930	0.000930	Constant
$\rho$ (kg m <sup>3</sup> )	998,207	998.207	Constant
$v(m^2 s^{-1})$	1.004E-06	1.004E-06	Constant
c(cm)	0.0125	0.0125	Constant
$\alpha$ (cm <sup>1</sup> )	0.0055	0.0055	Constant
Co	-6.344	-6.344	Constant
C1	-0.0000771	-0.0000771	Constant
C <sub>2</sub>	7.230E-10	7.230E - 10	Constant
C3	-0.685	-0.685	Constant
v (cm s <sup>-1</sup> )	104.22	103.35	Eq. (6)
$\tau_{av}(s)$	1.9	1.4	Eq. (5)
[dose]	104,298	102,602	Eq. (2)
$(\mu W s cm^2)$			
ln k	-6.5993	-6.5993	Eq. (1)
$(\mu W^{-1} s^{-1} cm^2)$			
$k(\mu W^{-1} s^{-1} cm^2)$	0.001361	0.001361	Eq. (1)
R <sub>c</sub> (dimension-	0.8263	0.8263	Eq. (7)
less)			
d (cm)	0.515	0.515	Eq. (8)
Re (dimension- less)	11,521	11,426	Eq. (11)
F (dimensionless)	0.0076	0.0076	Eq. (10)
$\delta$ (cm)	243.39	242.89	Eq. (9)
$\ln N/N_0$	-2.13	- 1.85	Eq. (3)
$\log_{10} N/N_0$	-0.92	-0.81	Eq. (4)
р		2.829	Eq. (12)

Comparison of traditional SVA with Fr 13 assessment for UV irradiation inactivation

of viable E. coli with DL-A kinetics in the presence of UV shielding agent with a % tolerance = 10% in turbulent flow in the annular reactor.

<sup>a</sup> Traditional single point, or, single value, assessment.

<sup>b</sup> One only of 10,000 scenarios.

<sup>c</sup> Values are reproduced from the r-MC sampling; it is not implied they need to be measured to this order.

#### 3. Results

Table 2 presents a comparison and summary of the traditional SVA with the new *Fr* 13 simulation of UV irradiation of viable *E. coli* for potable water with DL-A inactivation kinetics in the presence of UV shielding agent. UV key parameters are defined in column 1 of the table. The traditional SVA calculations are presented and read down column 2 where it is seen about 1-log<sub>10</sub> reduction (i.e. -0.92) in viable *E. coli* is obtained.

The *Fr* 13 simulation is summarised in column 3. In the absence of unconditional data, the distributions for the three key input parameters are defined by **RiskNormal** (mean, stdev), **RiskTruncate** (minimum, maximum). For example, for the suspended solids, [*conc*]=**RiskNormal** (0.115, 0.0023), **RiskTruncate** (0.1104, 0.1196) which defines a mean value=0.115 g L<sup>-1</sup>, with stdev=0.0023 g L<sup>-1</sup> and, respectively, (truncated) minimum and maximum, 0.1104 and 0.1196 g L<sup>-1</sup>.

For each of the key parameters it is seen in Table 2 that the truncated minimum and maximum values are defined by  $\pm 2 \times \text{stdev} (\text{stdev}=2\%)$  about the mean to imitate the most likely practical range of realistic values, and therefore outcomes for *p*. An advantage of using  $\pm 2 \times \text{stdev}$  on mean value is that 95% of all sampled values will fall in this interval (Sullivan, 2004; Vose, 2008). Notably, fluctuations in lamp intensity are also simulated with a truncated normal distribution. Lamp intensity will of course not be uniform with time but would be expected to fluctuate with

Table 3



Fig. 1. Distribution for the risk factor (p) from 10,000 scenarios of UV irradiation for inactivation of viable E. *coli* in the presence of UV shielding agent in turbulent flow in the annular reactor. Failure is defined for all p > 0.

age: it is not clear however whether this aging would in fact be uniform with time (Bolton and Cotton, 2008).

It is seen that the data of column 3 of Table 2 are for one-only Fr 13 scenario of the 10,000. All 10,000 are however summarized in Fig. 1.

A total 3205 failures were identified (32.1%). These can be seen in the right of the figure.

If each simulation is considered one operating day this translates to  $(3205/10,000 \times 12 \sim)$  four (4) surprise (unexpected) failures each calendar month, averaged over an extended period of operation due to the accumulation of combined naturally occurring random fluctuations in each of [conc], I<sub>0</sub> and Q. It cannot be assumed however these will actually be spaced evenly in time. Importantly however, this new insight is not provided by alternative current risk and hazard methodologies, with or without sensitivity analyses.

Twenty (20) of these 3205 failed scenarios are presented in Table 3. Row 4 (bold print) of the table highlights the particular failed scenario, and combination of parameters, presented in Table 2.

#### 4. Discussion

#### 4.1. Model confirmation

Model simulations were extensively tested and were shown to be stable. Given that predicted trends agreed with those published by Abdul-Halim and Davey (2015) over a wide range of inputs it was concluded the simulations were free of programming and computational errors and that the Fr 13 model was therefore suitable for the present purpose.

#### 4.2. Ability to identify each Fr 13 event

The advantage of the presentation of the data in Table 3 is that the particular combination of UV parameters that resulted in the failure can be readily identified. For example, in row 4 (bold print), the combination of  $I_0 = 54046 \,\mu\text{W cm}^{-2}$ ,  $[conc] = 0.115 \,\text{g L}^{-1}$  and  $Q=495.84 \text{ mL s}^{-1}$  (with corresponding p=2.829) can easily be read from the table. This ability to easily identify the values of the failure combination means Fr 13 simulations can be used to quickly screen process effects of key parameters, or impact of proposed interventions and physical changes to the plant.

Importantly, it is not implied that the numerical values given in Table 2 and, especially, Table 3, for Io, [conc] and Q (with corresponding p) would need to be measured to the stated value (the value is that randomly sampled and used in the r-MC simulations).

Twenty (20) selected failures from 3205 in 10,000 UV irradiation scenarios for UV shielding agent.

Row	$I_0 (\mu W \text{ cm}^2)^b$	[conc] (g L <sup>1</sup> ) <sup>b</sup>	Q (mL s <sup>-1</sup> ) <sup>b</sup>	р
1	54,493	0.117	497.96	0.066
2	55,430	0.112	507.03	0.969
3	54,480	0.116	499.05	1.903
<sup>a</sup> 4	54,046	0.115	495.84	2.829
5	55,048	0.115	505.36	3.703
6	56,184	0.116	516.02	4.533
7	54,814	0.112	504.63	5.479
8	53,985	0.117	497.57	6.288
9	54,835	0.118	505.97	7.426
10	54,938	0.116	507.71	8.456
11	54,942	0.118	508.44	9.466
12	54,076	0.116	501.53	10.544
13	54,347	0.113	505.08	11.818
14	53,973	0.112	502.79	13.108
15	54,655	0.118	509.79	14.492
16	54,657	0.117	511.04	15.871
17	54,661	0.113	512.71	17.615
18	54,428	0.113	512.09	19.289
19	53,842	0.115	508.88	21.685
20	53,256	0.117	519.74	36.385

Particular scenario of Table 2. Values are reproduced from the r-MC sampling; it is not implied they need to be measured to this order

Further, there is no rationale in the order of presentation of scenarios in Table 3, other than the lamp intensity value  $(I_0)$  is arranged from (row 1) greatest to (row 20) lowest, together with concomitant values of [conc], Q and p. It is not implied that this is the order the events would occur. The use of standard spread sheeting has meant the simulations have been logically ranked by machine from greatest to lowest.

#### 4.3. Impact of suspended solids

The predicted failure rate in UV efficacy because of the presence of suspended solids as shielding agent (Fig. 1) of 32.1%  $(k=0.00136 \,\mu W^{-1} s^{-1} cm^2)$ , averaged over the long term, is less than that for the failure rate for UV absorbing agent (k=0.00146  $\mu$ W<sup>-1</sup> s<sup>-1</sup> cm<sup>2</sup>) of 43.7%.

Nevertheless, with both shielding and absorbing solids, the predicted efficacy as log10 reduction in viable E. coli has been reduced to  $log_{10}\!\sim\!1$  from the  $log_{10}\!=\!4.35$  without suspended solids present and 16% failure rate reported by Abdul-Halim and Davey (2015). (This finding resonates with what would be expected).

Significantly, this reduction in viable pathogens falls below the level widely adopted in Regulatory guidelines of a minimum of 4log10 (i.e. 99.99%) (Anon. 2013: Sommer et al., 2008).

An advantage of the Fr 13 methodology however, is that it can be used in second-tier simulations (Abdul-Halim and Davey, 2015; Davey et al., 2015) to establish quantitatively the impact of changes to the physical system on its vulnerability to failure.

Repeat simulations to quantify the impact of the naturally occurring fluctuations about the mean, and maximum and minimum value, in each of suspended solids concentration as shielding agent, feed water flow, and lamp intensity on UV efficacy in the turbulent flow reactor were therefore carried out for a range  $1 \leq$ %-stdev  $\leq 10$ , % in the risk functions (Table 2). The risk function used was: RiskNormal (mean, stdev), RiskTruncate (mean- $-2 \times$  stdev, mean+2 × stdev) with respective means, [conc]= 0.115 g L<sup>-1</sup>, Q=500 mL s<sup>-1</sup> and  $I_0$ =55,400  $\mu$ W cm<sup>-2</sup>. Ten thousand (10,000) simulations were sufficient.

Results are summarized in Fig. 2.

The figure shows that with increasingly tighter control over the variance on the UV reactor parameters, implicit in the figure with



Fig. 2. Impact of %-stdev in distributions for combined, suspended solids as UV shielding agent [conc], feed water flow (Q) and lamp intensity (b), on the number of Pr 13 failures per 10,000 scenarios in UV irradiation of viable E. coli for potable water with DL-A inactivation kinetics in turbulent flow in the annular reactor.

#### Table 4

Spearman rank correlation coefficient (Snedecor and Cochran, 1989) for the three key input parameters of the annular reactor on UV risk factor (p).

Reactor parameter	Coefficient	
Q	+ 0.70	
I <sub>0</sub>	-0.68	
[conc]	+ 0.03	

deceasing values of %-stdev, the number of predicted Fr 13 failures decreases nearly exponentially. Tighter and tighter controls will become impractical in the limit however. At values greater than %-stdev ~8% however it is seen that the number of failures begins to plateau to a nearly constant value of 45/10,000 scenarios. However, it is important to note these predictions are for the combined effect of the three key reactor parameters,  $l_0$ , Q and [conc], on the UV risk factor, p.

To highlight the individual impact of each, the Spearman rank correlation coefficient (Snedecor and Cochran, 1989), readily available in @Risk, can be used, Table 4.

The data of Table 4 show that there is a strong correlation (+0.70) between the volumetric flow rate of water (Q, mL s<sup>-1</sup>) and p, and a strong inverse correlation (-0.68) with lamp intensity ( $I_0$ ,  $\mu$ W cm<sup>-2</sup>).

Conversely and unexpectedly however, it is seen there is a weak correlation (0.03) between suspended solids concentration ([conc], g L<sup>-1</sup>) and risk, p. That is, although there is an initial highly significant loss of UV efficacy because of suspended solids (respectively, 0.115 and 0.0115 g L<sup>-1</sup> for shielding and absorbing agent) the naturally occurring random fluctuation around this mean concentration in the feed water is not meaningfully impacting UV efficacy and vulnerability to survival of numbers of unwanted viable *E. coli*. The controlling parameter is seen to be the natural fluctuation in feed water flow to the reactor itself (together with fluctuation in lamp intensity).

#### 4.4. UV lamp intensity and dose

The effect of UV dose on the reduction of numbers of viable *E. coli*, with DL-A inactivation kinetics (Table 1), in the presence of UV shielding agent, [*conc*]=0.115 g L<sup>-1</sup>, in turbulent flow in the annular reactor is summarised in Fig. 3 for a range  $80,000 \le [dose] \le 120,000 \ \mu\text{W s cm}^{-2}$ .



Fig. 3. Impact of UV dose on reduction of numbers of viable *E. coli*, with DL-A inactivation kinetics, in the presence of UV shielding agent, [conc]=0.115 g L<sup>-1</sup>, in turbulent flow in the annular reactor.

It can be seen from the figure that in the presence of suspended solids as shielding agent a [*dose*]~119,800  $\mu$ W s cm<sup>-2</sup> is necessary to achieve the minimum, Regulatory (Anon, 2013; Sommer et al., 2008) reduction in viable *E. coli* of 4-log<sub>10</sub> (i.e. 99.99%). For the given UV lamp of intensity  $I_0$ =55,400  $\mu$ W cm<sup>-2</sup> this translates to a residence time of  $\tau$ =2.16 s necessary for inactivation of viable *E. coli* based on the extensive Amos et al. (2001) data. A direct comparison of these findings with independently

A direct comparison of these findings with independently reported values e.g. those of Sommer et al. (1998) and Parsons and Jefferson (2009) is problematic simply because these authors do not report the concentration, material (median particle size) or mechanism (as UV shielding/absorbing) of the suspended solids.

#### 4.5. Results overview

Practically applied, findings mean that random fluctuations in the feed water flow rate and lamp intensity (possibly increasing with age) have a more significant impact on vulnerability to failure to produce potable water in the annular UV reactor than fluctuations in the suspended solids concentrations as either UV shielding or absorbing, agents.

Ideally however, potable water that is free of suspended solids is a better outcome than extended UV treatment (dose), because these waters will retain (possibly unpleasant tasting and unsightly) suspended solids. Notably, suspended solids of particle sizes greater than about 40  $\mu$ m will be visible to the naked eye (Allen and Ansel, 2014; Anon, 2007). The UV shielding particles as *Celite 503* of Amos et al. (2001) simulated in this study with a median size 23  $\mu$ m are about 10 times greater than a typical coliform (Madigan et al., 2003; Anon, 2002) and are not visible to the naked eye. However, in the general case, many suspended solids of this size might impart unwanted taste(s) and odour(s).

A practical response therefore is for a regular and continuous monitoring of suspended solids (possibly using on-line analysers (Pernitsky and Muecci, 2002; Davis and Lettman, 1999)) in the feed water. With refined data and an iterative approach, secondtier simulations could then be readily used to guide engineering decisions on whether the introduction of a pre-filtration step for the feed water to a UV reactor was warranted.

Findings have been interpreted for a daily operation. With batch-continuous processes, say, daily pasteurisation of raw milk with Clean-in-Place (CIP) (Davey et al., 2015), each day can be reasonably thought of as 'one' event, however, UV irradiation for potable water is designed to be largely continuous.

In industrial application, at least two banks of parallel UV reactors would be needed to cover shutdowns and maintenance to give a continuous flow of potable water. A rationale therefore has been to assume a daily basis with a short-time for maintenance say a possible clean (there are essentially no moving parts) and replacement of the lamp bulb (at say 800 h). Another period however might be used, dependent on what further maintenance is actually required. On a monthly basis for example the reactor (s) might need to be shut down for bulb replacement. However because potable water is a critical utility, it is thought daily calibration checks would actually be needed. (There are strong parallels here with necessary daily operational checks on critical inline equipment such as industrial gas chromatographs, moisture analysers, etc).

Given that large-scale UV reactors are most likely housed inside a controlled environment (Ultraviolet Technology Australasia Pty Ltd., Australia, pers. comm.), it is not considered there will be any significant variations caused to the UV reactor parameters by seasonal change. In any event, the stdev and truncations on the distribution for solids concentration in the feed water [conc]= RiskNormal (0.115, 0.0023), RiskTruncate (0.1104, 0.1196) are designed to allow for feed water impacted by seasons. There are no UV parts sensitive to climate conditions (as these are generally quite robust).

Overall, a more unequivocal statement is that 32.1% of all operations would be expected to fail to produce potable water with the particular UV reactor over the long term.

To confirm the effectiveness of the predictions validation trials against independent literature data, or new data determined experimentally, are needed.

It is nevertheless concluded this work provides strong quantitative evidence for the removal of suspended solids prior to UV inactivation, together with precision control of the feed water flow; rather than an increased UV dose of waters containing suspended solids.

This research with continuous feed water containing suspended solids in a combined pre-treatment filter and UV irradiation reactor is presently under investigation (Abdul-Halim, 2015).

#### 5. Conclusions

The presence of suspended solids, as both UV shielding and UV absorbing agents, has a highly significant initial impact on decreasing the number of viable E. coli inactivated in feed water for potable water production in a continuous, turbulent flow 4series annular UV reactor. The predicted UV efficacy is reduced to approximately one log10 unit compared to 4.35 log10 units without suspended solids present in the same annular reactor.

The naturally occurring fluctuation in concentration of these solids in combination with lamp intensity (10) and feed water flow (Q) can result in some 32.1% and 43.7% of these continuous UV operations, over the long term, to fail to inactivate a ~1-log10 reduction in numbers of viable E. coli.

An unexpected finding, however, is that failure is impacted highly significantly by fluctuation in feed water flow rate and not fluctuations in concentration of solids in the water. It is the initial presence of suspended solids that reduces the practically achievable reduction in coliforms.

Practical validation trials against independent literature data or new data determined experimentally are needed however to confirm the effectiveness of the predictions.

It is concluded that pre-treatment of the feed water to remove (reduce) solids be used to exploit these findings, together with improved control to reduce fluctuation (variance) in the feed water flow to the annular reactor. The generalized model could be used for particular UV irradiation geometries to assess whether a pre-treatment for removal or reduction in solids would be warranted in production of potable water.

The work will be of benefit to operators of UV equipment and researchers in risk analyses.

#### Nomenclature

The number in parentheses after description is the equation in which the symbol is defined or first used.

- Correction constant for real reactor, cm (3)
- Model coefficients (1) C
- Suspended solids concentration,  $gL^{-1}(1)$ [conc]
- [dose] UV dose,  $\mu$ W s cm<sup>-2</sup> (2)
- Annular gap width, cm (8) d
- Friction factor, dimensionless (10)
- UV lamp intensity,  $\mu$ W cm<sup>-2</sup> (2) and (3) Inactivation constant,  $\mu$ W<sup>-1</sup>s<sup>-1</sup>cm<sup>2</sup> (1) I<sub>0</sub>
- k
- L
- Length of radiation section, cm (5) Concentration viable *E. coli*,  $mL^{-1}$  (3) and (4) N
- Concentration viable E. coli before UV exposure, mL-1 N (3) and (4)
- UV risk factor, dimensionless (12) p
- Volumetric flow rate, mL  $s^{-1}$  (6) 0
- Radius of inner cylinder, cm (6)-(8) R1
- Radius of outer cylinder, cm (6)-(8)  $R_2$
- Re Dimensionless group (7)
- Re Reynolds number, dimensionless (11)
- Average water velocity in annular gap, cm  $s^{-1}$  (6) v

#### Greek

- Absorption coefficient  $cm^{-1}$  (3)
- Boundary layer thickness, cm (3), (9) δ
- Dynamic viscosity of water,  $0.93 \times 10^{-3}$  kg m<sup>-1</sup> s<sup>-1</sup> (9) Density of water at 20 °C, 998.207 kg m<sup>-3</sup> (9) μ
- p
- Residence (exposure) time, s (2) and (5)
- Kinematic viscosity of water at 20 °C,  $1.004 \times 10^{-6}$ n  $m^2 s^{-1}(9)$

Other

Stolerance Practical tolerance (margin) in reduction in viable E. coli, % (12)

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