Intersection between engineering mechanics and supervised learning for modelling clogging dynamics in depth filters

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**Intersection between engineering mechanics and supervised
learning for modelling clogging dynamics in depth filters**

**CHEW WEI ZE, ALVIN
SCHOOL OF CIVIL AND ENVIRONMENTAL ENGINEERING**

2019

**Intersection between engineering mechanics and supervised
learning for modelling clogging dynamics in depth filters**

CHEW WEI ZE, ALVIN

School of Civil and Environmental Engineering

A thesis submitted to the Nanyang Technological
University in partial fulfilment of the requirement for the
degree of Doctor of Philosophy

Statement of Originality

I hereby certify that the work embodied in this thesis is the result of original research, is free of plagiarised materials, and has not been submitted for a higher degree to any other University or Institution.

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Supervisor Declaration Statement

I have reviewed the content and presentation style of this thesis and declare it is free of plagiarism and of sufficient grammatical clarity to be examined. To the best of my knowledge, the research and writing are those of the candidate except as acknowledged in the Author Attribution Statement. I confirm that the investigations were conducted in accord with the ethics policies and integrity standards of Nanyang Technological University and that the research data are presented honestly and without prejudice.

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Associate Professor LAW WING
KEUNG, ADRIAN

Authorship Attribution Statement

This thesis report contains material from 9 papers published in the following peer-reviewed journals and from papers accepted at conferences in which I am listed as an author.

The contents in Chapters 1 to 8 contain the following papers, namely: (a) 6 peer-reviewed journal publications (5 accepted versions, 1 currently under review); and (b) 3 peer-reviewed conference publications (accepted versions)

1. **Chew, A. W. Z., & Law, A. W. K.**, Modelling clogging dynamism within dual-media pre-treatment rapid filters in seawater desalination, ***Energy Procedia***, 143, 466-474, 2017. DOI: <https://doi.org/10.1016/j.egypro.2017.12.712>
2. **Chew, A. W. Z., & Law, A. W. K.**, DRFM hybrid model to optimize energy performance of pre-treatment depth filters in desalination facilities. ***Applied energy***, 220, 576-597, 2018a. DOI: <https://doi.org/10.1016/j.apenergy.2018.03.028>
3. **Chew, A. W. Z., & Law, A. W. K.**, Multi-scale homogenization of pre-treatment rapid and slow filtration processes with experimental and computational validations, In: Shi Y. et al. (eds) Computational Science – ICCS 2018. ICCS 2018. ***Lecture Notes in Computer Science***, 10861. Springer, Cham, 2018b. DOI: https://doi.org/10.1007/978-3-319-93701-4_66
4. **Chew, A. W. Z., Vu, T. T. & Law AWK.**, High Performance Computational Hydrodynamic Simulations: UPC Parallel Architecture as a Future Alternative, In: Shi Y. et al. (eds) Computational Science – ICCS 2018. ICCS 2018. ***Lecture Notes in Computer Science***, 10860. Springer, Cham, 2018. DOI: https://doi.org/10.1007/978-3-319-93698-7_34

5. Vu, T. T., Law AW-K., Nguyen T. H., **Chew, A. W. Z.**, Computational flood modelling with UPC architecture, ***Computing in Civil Engineering, ASCE***, vol. 33 (2), 2018. DOI: [https://doi.org/10.1061/\(ASCE\)CP.1943-5487.0000811](https://doi.org/10.1061/(ASCE)CP.1943-5487.0000811)
6. **Chew, A. W. Z.**, & Law, A. W. K., Feature engineering using homogenization theory with multiscale perturbation analysis for supervised model-based learning of physical clogging condition in seepage filters. ***Journal of Computational Science***, v32, 21-35, 2019a. DOI: <https://doi.org/10.1016/j.jocs.2019.02.003>
7. **Chew, A. W. Z.**, & Law, A. W. K., Homogenization theory with multiscale perturbation analysis for supervised learning of complex adsorption-desorption process in porous-media systems. ***Journal of Computational Science***, 40, 101071. 2020. DOI: <https://doi.org/10.1016/j.jocs.2019.101071>
8. **Chew A.W.Z.**, & Law, A. W. K., Multiscale grid representations of deep neural layers for modelling complex engineering processes, 2020 (Under Review). ***International Journal of Machine Learning and Cybernetics***, **Selected for full paper extension from recent conference proceedings at CCIS 2019.**
9. **Chew, A. W. Z.**, Law AW-K., Vu, T. T., Optimizing Performance of Computational Hydrodynamic Simulations with UPC Programming Model, ***Computing in Civil Engineering, ASCE*** 34(2), 06020001. DOI: [https://doi.org/10.1061/\(ASCE\)CP.1943-5487.0000876](https://doi.org/10.1061/(ASCE)CP.1943-5487.0000876)

My contributions to papers 1, 2, 3, 6, 7 and 8 are as follows:

- I performed all analytical derivations and simulation runs for training and testing the machine learning models built.
- I prepared the experimental materials and performed the analysis.
- I prepared all manuscripts (writings, figures plots, tables, etc.).

The contributions to papers 1, 2, 3, 6, 7 and 8 by the co-authors are as follows:

- Associate Professor Adrian Law provided the initial project directions, checked on my analytical derivations and analyses, and edited the manuscripts.

My contributions to papers 4, 5 and 9 are as follows:

- I worked with Vu, T. T., who is the second, first and third author of papers 4, 5 and 9 respectively to build the algorithm for the computational model built in both papers. We performed the analyses together.
- I prepared all manuscripts (writings, figures plots, tables, etc.,) for papers 4 and 9.
- I co-authored the manuscript (writings, figures plots, tables, etc.,) for paper 5.

The contributions to papers 4, 5 and 9 by the co-authors are as follows:

- Vu, T. T., who is the second, first and third author of papers 4, 5 and 9 respectively, worked with me to build the algorithm for the computational model built in both papers. We performed the analyses together.
- Associate Professor Adrian Law provided the initial project directions, checked on the analyses, and edited the manuscripts.

18.Feb.2020

Date

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LIST OF SYMBOLS

A_g	BET surface area per unit mass of media grains
A_j	Vector function
$A_{monolayer}$	Surface area of monolayer packing around the spheres' boundaries respectively within each cell domain
$A_{spheres}$	Surface area of ideal collector spheres within each cell domain
A	Lumped coefficient for physical clogging problem in (3.3.11)
α_1	Learning rate hyperparameter
α_2	Size of mini batch hyperparameter
α_3	Number of epochs hyperparameter
α	Lumped coefficient for chemical clogging problem in (7.1.1)
B	Lumped coefficient for physical clogging problem in (4.1.2)
β	Respective lumped coefficient for physical and chemical clogging problem in (3.3.4) and (3.4.16) respectively
c_0	Initial concentration of influents
C_1, C_2	Arbitrary constants for (5.2.3)
C	Biased term for regression model in Tables 7.3.5a and 7.3.5b
c_s^*	Concentration at collector sphere's boundary
c_s	Dimensionless concentration at collector sphere's boundary
c^*	Concentration
c	Dimensionless concentration
c_{eqm}	Equilibrium dimensionless concentration
D_p^*	Diffusion coefficient
$D_{a,L}$	General macroscale Damköhler number
$D_{ads,L}$	Macroscale Damköhler number for adsorption reaction
$D_{c\%}$	Clogging degree
$D_{des,L}$	Macroscale Damköhler number for desorption reaction
D_p	Particle diffusivity scale
d^*	Diameter of collector spheres
d_0^*	Initial diameter of media grains
d	Dimensionless diameter of collector spheres
d_c	Growing diameter of collector spheres in DRFM model
d_p	Average diameter of particle/contaminant
$E_{savings}$	Total energy savings gained from the difference between S1 and S2 with respect to S1
E_{total}	Total energy cost to per unit volume of filtrate
E_t	Average kilowatt-hour required to effectively filter per unit volume of influent
F	Theoretical filter capacity
G	Fluid parameters
g	Constant gravitational acceleration

H_0	Filter's initial energy loss incurred at $t = 0$
H_t	Filter's energy loss incurred at dimensionless time (t)
J	Filter's hydraulic gradient
k	Reaction rate parameter
$\tilde{k}_{ij}$	Effective permeability tensor
$\tilde{k}$	One-dimensional average permeability coefficient
k_{abs}	Absorption rate of contaminants
k_{ads}	Adsorption rate of contaminants
k_{des}	Desorption rate of contaminants
k_{det}	Detachment rate of contaminants
k_{rem}	Removal rate of contaminants
L_m	Media depth
L	Characteristic macroscale media depth
l	Characteristic microscale grain size
M_{GHG}	Mass of GHG gases measured in carbon dioxide equivalents
m	Lumped coefficient for physical clogging problem in (3.3.11)
N	Number of instances in (5.2.4) – (5.2.6)
n_1, n_2	Arbitrary constants for (4.1.4)
Pe_l	Microscale Peclet number
Pe_l'	Macroscale Peclet number
P	Pressure scale
p^*	Fluid pressure
p	Dimensionless fluid pressure
Q_{in}	Inlet flowrate
q_{in}	Inlet hydraulic loading rate
Re_l	Microscale Reynolds number
S^*	Sphere's boundary
S1, S2	Scenarios 1 and 2 for energy cost analysis in Section 7.4.1
T_c	Convection time scale
T_{ads}	Adsorption time scale
T_{des}	Desorption time scale
T_{abs}	Absorption time scale
T	Time scale
t^*	Time
t	Dimensionless time; throughput units
t_b	Dimensionless breakthrough time of depth filter
U	Velocity scale
u^*	Velocity vector
u	Dimensionless velocity vector
V_b	Volume of backwash waste
V_f	Volume of filtrate
V_s	Superficial velocity/Inlet flow velocity

w	Angular frequency of periodic functions
X	Lumped representation of (5.2.3)
x^*	Position vector
x	Dimensionless position vector
Y_{obs}	Measured/observed target values
Y_{pred}	Predicted target values
z	Variable filter depth
ε_c	Porosity of rapid depth filter during physical clogging stage
ε	Dimensionless length scale; small perturbation parameter
$\tilde{f}$	Average quantities
l	Microscale length
η_I	Removal efficacy due to interception
η_G	Removal efficacy due to gravitational sedimentation
η_c	Filter's effective removal efficacy under clogging conditions
ρ_p	Bulk density of turbidity particles
ρ_s	Density of influent being filtered for energy cost analysis in (7.4.2)
ρ_w	Density of fluid
μ	Pore-scale separation between media grains in periodic cell domain
μ_{in}	Dynamic viscosity of fluid
ν	Kinematic viscosity of fluid
Ω_f	Fluid phase inside periodic cell
$ \Omega_f $	Volume of fluid inside periodic cell
Ω_{fs}	Interface between solid and fluid phases inside periodic cell
Ω_s	Solid phase inside periodic cell
Ω	Periodic cell
$ \Omega _V$	Volume of periodic cell
δ_{ij}	Kronecker delta
γ	Assumed porosity of a monolayer packing of contaminants in the fluid phase around the grain/sphere surface
σ	Specific deposit
θ'_A	Fixed length scale adopted in DRFM
θ	Periodic cell's porosity
ϕ	Unknown effluent discharge concentration profile at the maximum media depth
π_i	Dimensionless pi-terms; $i = 1, 2, 3, \dots$
$(\Delta H)_t$	Filter's direct energy gradient incurred over time (dimensionless quantity) due to effective clogging
∇S^*	Outward normal vector acting upon collector sphere's boundary

SUMMARY OF THESIS

Granular depth filtration technology is widely deployed in many water-related infrastructures, which include water and wastewater treatment plants, desalination facilities, natural and engineered aquifers, with the focus objectives of providing potable water to communities and/or to pre-treat contaminated feedwater prior to further treatment processes in engineering plants. Notwithstanding the dominance and conventionality of the depth filtration technology, effective quantifications of the complex clogging dynamics continue to be a hindrance for predictive maintenance actions by field engineers today. To address this problem statement, this thesis study innovates on traditional engineering techniques, specifically engineering mechanics, dimensional analysis and supervised machine learning algorithms, to build novel predictive tools to model complex clogging conditions, of physical and chemical characteristics, in operating depth filters under varying flow conditions, i.e. microscale filtration Reynolds numbers. Measured data, as extracted from previous studies and experimental runs carried out in this study, are then leveraged to calibrate the proposed engineering models to encapsulate the real-world complexity of the clogging problem inside the filters. Following which, quantitative and qualitative details are provided to demonstrate the predictive capabilities of the calibrated models for the predictive maintenance objective, which can serve as useful results for field engineers in adopting the hybrid engineering approach as proposed in this thesis study for other important environmental and chemical engineering applications. Finally, details are also provided about the author's present research study to build engineering tools, using the same modelling methodology from that of the physical and chemical clogging conditions, to quantify the complex biological clogging behavior inside depth filters for the same target objective. Succinct details about innovating the proposed engineering approach further are also put forth.

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Chapter Overview:

This chapter first describes the high-level details associated with the granular depth filtration technology deployed in many water-related infrastructures on the industry scale which constitutes to the background context of this thesis study. Following which, low-level details of the identified problem statements for the different types of filtration technologies are provided extensively. Finally, the exact objectives of this thesis study together with the respective technical scope are delineated clearly to the readers.

Section 1.1 provides the contextual overview of operating the different types of granular depth filtration technologies on the industry scale, followed by qualitatively describing the present difficulties faced by field engineers in Section 1.2 which thus establish the key problem statements in this thesis study. Section 1.3 describes the study objectives together with the exact scope of details to be covered in this thesis.

1.1. Background information

Today, granular depth filtration is a dominant purification technology deployed in many water-related infrastructures on the industrial scale which include water treatment plants, wastewater treatment plants, natural and engineered aquifer recharge and recovery systems (ARRS) and seawater reverse osmosis (SWRO) desalination facilities. For example, in both water and wastewater treatments facilities, pre-treatment depth filters containing porous media such as sand, coal and gravel are commonly deployed to remove pathogens and suspended solids (Darby et al., 1991; Williams et al., 1997; Crittenden et al., 2012). Molinos-Senante et al. (2018) and Velasquez-Orta et al. (2018) recently demonstrated the energy efficiency advantages provided by biological filters in existing activated sludge treatment plants. In many medium- and large-scale SWRO desalination plants, pre-treatment depth filters are responsible for removing turbidity particles and natural organic matter (NOMs) from seawater influents to mitigate fouling in the downstream reverse osmosis (RO) membranes (Voutchkov, 2012; Voutchkov, 2017a; Anis et al., 2019). This pre-treatment step typically consumes around 10% of the total specific energy cost for operating SWRO desalination plants, which is currently $\sim 4.0 \text{ kwh/m}^3$ on average, under normal operating conditions (Voutchkov, 2018).

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To ensure high production rate of purified water in large-scale treatment facilities, depth filters are usually rapid driven either by mechanical (pressure) or gravity forces. Molinos-Senante and Sala-Garrido (2017) underlined the importance of rapid gravity filters to provide economies of scale (EOS) in the energy intensities of water treatment plants respectively. Their findings emphasized the energy-associated benefits offered by depth filters in water-related infrastructures. Most recently, Molinos-Senante and Sala-Garrido (2018) confirmed that rapid-gravity depth filtration technology, coupled with coagulation-flocculation processes, provides the highest energy efficiency for water treatment plants by using a novel energy efficiency score which combines the filter's energy intensity (consumption) and pollutant removal metrics. Hence, there is optimism that conventional depth filtration technology can contribute to the overall energy savings of operating large-scale water industries (desalination, water-treatment, etc.). The embodied energy cost of a typical rapid filtration process can generally be sub-grouped into direct and indirect energy cost components (Wakeel et al., 2016), whereby the former arises from the rapid filtration and the backwashing (filter maintenance phase) steps while the latter derives from chemicals usage and administrative services incurred from the maintenance act (Mo et al., 2011).

At present, there is an average global demand of 86.8 million cubic metres of desalinated water daily (IDA, 2018). Therefore, significant amount of energy is required to operate medium- and large-scale SWRO desalination plants globally which thus contributes to climate change via the emissions of greenhouse gases (GHG), etc (Facchini et al., 2017). Studies have also confirmed that each unit volume of desalinated water consumes the most energy among other water technologies (Voutchkov, 2018). This relationship between the volume of desalinated water produced and the required energy usage can broadly be termed as water-energy nexus (Dubreuil et al., 2013; Wakeel et al., 2016; Lee et al., 2017). The above-mentioned EOS advantage (Molinos-Senante and Sala-Garrido., 2017) provided by rapid depth filters in water treatment and desalination plants can thus be useful to offset a portion of the total energy cost incurred by the operating plants via extended production rate of filtrate daily. Directly, this optimal practice can be achieved via predictive maintenance which has been shown to provide both economic and environmental benefits for engineering operations (Mobley, 2002). On a whole, the

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predictive maintenance act involves pre-estimating, with sufficiently high level of confidence, the optimal timings to perform maintenance of depth filters in treatment facilities. By doing so, the following key advantages can : (a) minimize logistical problems by obviating unexpected downtime of filters; (b) derive long-term energy savings via the EOS effect; and (c) minimizing the frequency of maintenance which directly reduces the total amount of sludge or waste produced per unit filter.

While SWRO desalination technology continues to be a dominant option in providing potable water, ARRS systems are gaining increasing popularity as an alternative supply, particularly in arid locations, near coastal regions and regions having significant wet and dry weather conditions (Bloetscher et al., 2014; Masciopinto et al., 2017; Jeong et al., 2018). The key advantages of ARRS (Bouwer, 2002; Masciopinto et al., 2017; Jeong et al., 2018) over SWRO technology are namely: (a) providing natural pre-treatment of stormwater infiltrations with minimum energy requirements; (b) minimizing seawater intrusions hence mitigating land subsistence; (c) minimizing evaporation rates of stormwater collections; and (d) storing large volumes of stormwater for future and emergency uses. While both are similar functionally, the filtration velocity range between ARRS and pre-treatment depth filters in SWRO desalination plants differs greatly. As discussed, rapid depth filters deployed in desalination plants have the microscale filtration Reynolds number, which measures the ratio between the inertial and viscous forces of the fluid within the pore spaces of the porous media system, greater than the value of unity (MWH, 2005). On the contrary, ARRS can be analysed as seepage depth filters and have microscale filtration Reynolds number much smaller than the value of unity (MWH, 2005), thus leading to creeping flow conditions inside the global pore spaces of the filters.

In both rapid and seepage depth filters, clogging of the available pore spaces gradually materialise during operations as different types of contaminants are removed from the influent feedwater for producing cleaner effluents over time. The clogging behaviour can generally be grouped into physical, chemical and biological characteristics. Physical clogging is mainly triggered by the transient trapping of suspended solids and physical impurities within the filter's pore spaces via interception, straining and gravitational sedimentation mechanisms broadly (Yao and O'Melia., 1968; Yao et al., 1971; MWH, 2005), while chemical clogging is the result of

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prolonged precipitation of sub-microns contaminants from the filter's fluid phase and their subsequent adsorption onto the impermeable surfaces of the media grains inside the filter (Jeong et al., 2018). Finally, biological clogging is caused by the transient development of a complex biofilm layer around the irregular surfaces of the media grains due to continuous consumption of biodegradable organics and other contaminants by the residing microbes at the media surfaces (MWH, 2005; Jeong et al., 2018).

1.2. Problem statements

Prolonged clogging (physical, chemical or biological) of depth filter systems requires periodic maintenance to restore their original clean state for continuous effective filtration performance. In the following, details are provided for the maintenance actions performed for filters undergoing the different clogging conditions, and the present problems faced by field engineers to achieve predictive maintenance.

For managing the physical clogging condition, the focus is on both rapid and creeping flow conditions inside depth filters. In the former scenario, maintenance is performed by shutting down the rapid filters' operations followed by backwashing with filtered water or/and air scouring for a defined period (MWH, 2005; Crittenden et al., 2012; Voutchkov, 2017a). The maintenance action is typically initiated upon detecting either of the following criteria under constant-flux operating conditions: (a) direct energy cost incurred by operating filters, in terms of the elevation head above the media surface, exceeds a defined threshold value during operations; or (b) sudden rise in the effluent turbidity concentration due to significant detachment of the initially trapped contaminants inside the filter. Typically, rapid filters require between 2.0m to 3.8m in terms of the elevation head for normal operations. This threshold range can, however, be quickly exceeded during the treatment of high-turbid influents, i.e. having the turbidity concentration of greater than 50 NTU (WHO, 2004), due to accelerated clogging rate of the filter's pore spaces during its effective filtration stage. However, accurate predictions of the timings for any arbitrary rapid filter to reach its maximum clogging capacity when treating low- and high-turbid influents remains computationally challenging till today.

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Maintenance of seepage depth filters (ARRS), under creeping flow conditions, is instead performed via scrubbing, well jetting, vacuum pumping (Martin, 2013; Jeong et al., 2018), mechanical surging and heating (Driscoll, 1986; Martin, 2013) which can be more expensive and time-consuming than that of rapid depth filters. In this scenario, maintenance is initiated when the seepage filter's global permeability coefficient reaches a stagnated state for a period (breakthrough stage) under constant-pressure operating conditions. In events of sudden breakthrough, logistical problems occur which can adversely affect the supplies of potable water, especially in arid regions. At present, field engineers are unable to estimate a priori the timings for both rapid and seepage depth filters to reach their respective breakthrough stages due to an incomplete quantitative understanding of the complex physical clogging dynamics taking place inside the filters. Reactive maintenance is still the common practice by engineers which may not be operationally optimal and can lead to logistical issues. Fixed scheduled maintenance is also not ideal in scenarios whereby clogging is still relatively minimum inside the operating filters which directly hinders any possibility of extended production rates of filtrate during operations.

The above discussed difficulties underline the need for an engineering tool which can accurately quantify the physical clogging rate occurring inside depth filters, under different flow conditions, at a relatively early stage of operations and then extrapolate the continuous clogging effects on the filters' final breakthrough time as a function of the known operating parameters. By doing so, predictive maintenance of both rapid and seepage depth filters can be performed. Development of the desired predictive models requires engineers to first effectively quantify the complex packing of the porous media on the filters' physical clogging rate over time and then using supervised learning methods for model calibration with measured data. This thus constitutes the key problem statement in this thesis study for modelling physical clogging condition in both rapid and seepage depth filters.

For seepage depth filters which undergo either chemical or biological clogging conditions over time, exhaustion of their deployed media occurs when the filters' effluent concentration of contaminants exceeds a pre-defined threshold value. Subsequently, the deployed media must be reactivated (Driscoll, 1986; Hajra et al., 2002) via appropriate treatment processes at local treatment plants before

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redeployment. One common treatment process is via high-temperature pyrolysis which results in the forced desorption of the previously adsorbed (chemical clogging) or absorbed (biological clogging) contaminants from the media surfaces (San Miguel et al., 2001; Benstoem et al., 2017). The above listed maintenance practices are again expensive operationally and labour-intensive due to the need to remove the exhausted media from depth filters and be transported to the treatment plants. Unexpected exhaustion of the operating filters is again adverse as it leads to logistical problems during reactive maintenance. Hence, predictive maintenance is again desirable to obviate the described problem which is again difficult to achieve without an engineering tool which can encapsulate the transient dynamics of either the chemical or biological clogging condition taking place in depth filters.

The primary reason for the missing engineering tool at present is due to the challenge of quantifying the complex adsorption/absorption and desorption processes taking place concurrently inside depth filters. During the filter's initial operational stage, changing absorption/adsorption and desorption rates of contaminants are occurring at the media surfaces of relatively clean state due to varying transient concentration gradient of contaminants from the fluid phase to the same surfaces. Over time, the concentration of contaminants at the media surfaces increases which inhibits further absorption/adsorption, and desorption flux of the initially adsorbed/absorbed contaminants back into the fluid phase in the reverse direction becomes increasingly important. Developing an engineering model, via analytical means, to quantify the above-described complex concentration dynamics then sets up the key problem statement for modelling both chemical and biological clogging conditions inside depth filters.

1.3. Scope and objective of Ph.D. study

This thesis aims to develop new engineering approaches to model the complex physical, chemical and biological conditions in depth filters for building towards the predictive maintenance objective. Explicitly, novel methodologies by leveraging on analytical and numerical techniques are proposed to quantify the dynamics inherent to the different clogging problems and then verified accordingly to justify the new

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approaches. This thesis study first leverages on advanced engineering mathematical methods, specifically the homogenization theory coupled with the multiscale perturbation analysis, to develop homogenized averaged representations which can encapsulate the complex clogging dynamics in depth filters under creeping flow conditions. Before which, the significance of coupling the homogenization theory with the multiscale perturbation analysis is first discussed, followed by describing the respective strengths and shortcomings of the proposed technique.

For generality, the homogenization theory studies partial differential equations (Navier-Stokes, Einstein conservative forms, etc.) having rapidly varying coefficients whereby those coefficients vary rapidly at the different scaling of importance associated with a very small perturbation parameter defined a priori. The perturbation parameter is defined as the ratio of the defined quantities (length, volume, etc.) between the microscale and macroscale domains associated with the problem. The proposed hybrid technique derives average homogenized representations which quantify the macroscale behavior with a sufficiently small periodic microstructure (Papanicolaou and Bensoussan, 1978; Sánchez-Palencia, 1980; Hornung, 2012; Battiato et al., 2019), which is again linked to the same defined perturbation parameter. Within each periodic microstructure, i.e. cell problem, the perturbation analysis involves a well-known volume averaging method to average the microscale variations of the physical parameters such as concentration, velocity etc., by adhering to the defined perturbation parameter for their asymptotic expansions. Systematically, the average macroscale behavior is approximated by summing up the respective homogenized values or expressions, via volume averaging, at the different scales till the desired error accuracy is attained.

While the periodic cell problem is not a realistic assumption, and may not be entirely correct mathematically, the hybrid approach is useful to garner first approximations of the complex macroscale behavior relating to the analysed problem. For example, in porous media systems, the proposed technique derives the averaged effective representations for the fluid and mass transport parameters which include diffusion, velocity, concentration, pressure, etc., which will be demonstrated in the later sections. To apply the hybrid technique to the any specific problem, the modeller must effectively define the different scales affiliated to the concerned problem for setting up

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the most appropriate perturbation parameter to derive the required macroscale parameters, via the multiscale perturbation analysis, for useful engineering predictions. Generally, the advantages and shortcomings of the hybrid technique can be summarized as follows:

Advantages:

- Easy reproducibility of the homogenized representations for the respective problems due to the formal elegance of the multiscale perturbation analysis and the use of clear, traceable, logical and exhaustive assumptions.
- Rigorously derived from consistency arguments, hence placing less emphasis on domain knowledge to derive the homogenized representations for engineering predictions.

Shortcomings:

- Debate over the sole use of the periodic microstructure to quantify the macroscale behavior which may not capture non-local behaviours in regions where the small perturbation parameter and homogenization assumption break down.
- Difficult to derive exact analytical solution to capture highly non-linear behavior at the macroscale which can be important for very complex engineering problems.

In this thesis study, the homogenized representations, as derived from the above-discussed hybrid approach, are useful to reduce the feature space responsible for quantifying the complex clogging behaviours of varying characteristics in depth filters. Fundamental dimensional analysis, via the Buckingham pi-group theorem, is subsequently performed to analyse the reduced feature space as a function of the known physical parameters for predictive analysis. For each specific clogging behavior under creeping flow conditions, the derived dimensionless equation contains unknown coefficients which can be calibrated via supervised learning methods with an augmented pool of measured data from the literature. The calibrated equation can then be useful to extrapolate the timing for the depth filter to reach its respective breakthrough phase for predictive maintenance.

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The second core focus of this thesis is to build personalized computational predictive tools, namely: (a) dynamical rapid filtration model (DRFM); and (b) recurrent neural network coupled with long-short-term-memory cells (RNN-LSTM), which can model the complex physical clogging behavior in depth filters under rapid flow conditions. Both DRFM and RNN-LSTM are expected to effectively quantify the direct energy gradient cost incurred by rapid filters during their effective clogging of turbidity particles in the intake feedwater. Comparison between DRFM and RNN-LSTM of their respective forecasting accuracy with suitable cost-functions is later carried out to determine which of the two proposed models is most appropriate to achieve the predictive maintenance objective for providing long-term energy savings and GHG reduction, particularly for large-scale rapid filter facilities.

The pre-processed feature space of both DRFM and RNN-LSTM are again built, via dimensional analysis, with the Buckingham pi-group theorem of the commonly reported physical parameters which can affect an arbitrary rapid filter's direct energy gradient due to effective physical clogging. Raw measured data associated with rapid filtration experiments, as derived in this thesis study and previous experimental works, are then appropriately augmented to build a larger pool of training instances for verifying the predictive capabilities of DRFM and RNN-LSTM accordingly. After which, the present analysis provides the quantitative and qualitative details of the economic and environmental benefits garnered from the predictive maintenance act of rapid filters by the best numerical model.

This thesis report is structured as follows and illustrated in Figure 1.3.1. Chapter 2 extensively discusses the previous research works done to model the different clogging behaviours in porous media systems (depth filters). A focus section in the same chapter will be directed towards previous analyses done using the homogenization theory with multiscale perturbation analysis to model the flow and mass transport behavior in porous media systems, and the respective strengths and shortcomings of those models. Chapter 3 innovates the proposed hybrid analytical approach to model the physical and chemical clogging conditions in depth filters under creeping flow conditions, followed by describing the pre-processing technique in Chapter 4 to couple the proposed theoretical models with supervised learning methods

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in this thesis study. Chapter 5 provides the developmental details of both DRFM and RNN-LSTM to model the physical clogging behavior in depth filters under rapid flow conditions. Chapter 6 describes the experimental studies carried out in this thesis study to enlarge the pool of training instances for modelling the different clogging conditions in depth filters. Chapter 7 extensively discusses the results derived from the proposed models for the predictive maintenance act of the depth filters undergoing specific clogging behavior (physical and chemical characteristics) under varying flow conditions. Chapter 8 succinctly describes the focus and derived outcomes from this thesis study, followed by describing the quantitative and qualitative details of the engineering model, at its preliminary phase, which is built to quantify the complex biological clogging condition in depth filters. Details for model improvements, which constitute to future research studies, are also described in the same Chapter.

Figure 1.3.1. Contents flow in present Ph.D. thesis.

Chapter Overview:

Systematically, this chapter first describes the previous works done in leveraging the coupled homogenization theory with multiscale perturbation analysis to model the flow and mass transport behavior in porous media systems, followed by discussing the respective strengths and shortcomings of those models and how the proposed methodologies adopted in this thesis study differ from previous studies to model the different clogging conditions. The chapter then proceeds to discuss previous models built, via analytical, computational or experimental means, to quantify the complex clogging behavior of physical, chemical and biological characteristics taking place inside depth filters under varying flow conditions.

Section 2.1 provides the details of previous studies done in adopting the coupled homogenization theory with multiscale perturbation analysis to model the flow and mass transport behavior in porous media systems. Chapters 2.2 to 2.4 discuss the previous modelling works done to respectively quantify the physical, chemical and biological clogging conditions in depth filters under varying flow conditions.

2.1. Homogenization theory coupled with multiscale perturbation analysis for modelling flow and mass transport behavior in porous media

Papanicolau and Bensoussan (1978) and Sánchez-Palencia (1980) provided extensive quantitative details of leveraging the homogenization theory with multiscale analysis for a wide-range of periodic or near-periodic structures. Their work has since served as a basis for many important research studies to analyse the complex fluid flow and mass transport problems in porous media domains by adhering to either periodic or near-periodic microstructure for simplifying the complex analysis. One prominent example is the works by Mei et al. (1996) and Mei and Vernescu (2012a) which adopt Navier-Stokes flow representations and mass balance principle to model the macroscale hydraulic conductivity, i.e. permeability, in saturated porous media systems for engineering predictions. The authors adhered to a periodic cell domain of arbitrary packing configuration and used advanced calculus techniques to rigorously derive homogenized representations for the permeability parameter. Following which, Mei and Vernescu (2012b) leveraged on their previous work (Mei et al., 1996; Mei and Vernescu, 2012a) to model the complex dispersion coefficient in porous media

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systems (Mei, 1992) which again involved a significant amount of engineering mathematics to demonstrate the novelty of the analytical approach. Their work is one of the must-read for readers interested in using the proposed homogenization theory and multiscale perturbation analysis for engineering modelling.

Building upon the above works, significant amount of analytical studies has been carried out to model the mass transport behavior of different types of contaminants inside spatially periodic domains by rigorously deriving exact convective-dispersion equations, while incorporating novel reactive processes in some of those studies. Ng and Mei (1996a) systematically derive the homogenized representation to govern the convective diffusion of volatile organic compounds. Their work can be extended to three-scaled media system. In addition, their study confirmed that microscale equilibrium is attained when the diffusion time inside the pore-spaces is greater than the flow advection time at the macroscale which can be important information for modelling chemical and biological clogging conditions in porous media, as demonstrated later in this thesis study. In their subsequent work (Ng and Mei, 1996b), the authors adopted their previously derived model to quantify vapor transport in one-dimensional filter column by comparing the engineering predictions with previously measured data. In a similar work, Lee et al. (1996) extended the mathematical methodology to model the permeability and dispersion coefficients of heat transfer mechanism in porous media system. Their work was more rigorous mathematically due to need to account for the energy balance in thermodynamic processes, which is often neglected in fluid flow systems.

Other novel contributions involve the coupling of the hybrid analytical technique with other numerical and/or approximation methods. For example, Xu and Meakin (2013) and Chamsri and Bennethum (2015) coupled the Fourier series analysis and finite element method respectively with the multiscale analysis to study the flow and mass transport for different periodic structures. Their methodologies further improve on the multiscale analysis approach for engineering predictions of the complex permeability and dispersion coefficients in porous media systems. Most recently, Wang et al. (2018) adopted the multiscale method to perform a coarse-grained grid analysis of the hidden neurons in deep neural networks for computing the flow dynamics parameters and diffusion coefficient inherent to mass transport problems.

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Their methodology is novel as the multiscale model reduction method provides a refined feature space for computations which thus helps with model training for data-deficiency cases and reduces the total training time for model calibration. In a more specific application to porous-media system, Wang and Sun (2018) extensively coupled the multiscale and homogenization methods with deep learning and suitable numerical simulations to model hydro-mechanical coupling effects of porous media with pores having a range of sizes. Their impressive work has since opened new dimensions to leverage numerous types of simulations and measured data across the multiple length scales (macroscale, microscale, etc.) for supervised learning methods. On a whole, these recent novel research works underline the usefulness of the multiscale analysis to be coupled into machine learning algorithms to improve the engineering predictions for complex processes, which align with the core focus of this thesis study.

For analysing the clogging behavior in porous media systems, researchers have developed new ideas in adopting the same analytical technique to predict the complex clogging rate in depth filters. One good example was the recent publications of several insightful works by a research team in Oxford University, Mathematical Institute, which details will be described as follows. Firstly, Dalwadi et al. (2015) demonstrated in quantitative details the effectiveness of a decreasing porosity gradient along the media depth to maximise any arbitrary filter's trapping capability. Their results make intuitive sense as significant amounts of contaminants tend to be trapped within the filter's upper compartments, which is close to the entrance of the influent suspensions, during operations. This observation will also be validated in the proposed dynamical rapid filtration model (DRFM) later in this thesis study and has also been confirmed in most recent studies (Chu et al., 2019). In their subsequent work (Dalwadi et al., 2016), the authors built upon their previous model (Dalwadi et al., 2015) to account for the clogging effects by assuming a first-order reaction mechanism on the surface of a singular sphere inside a regular periodic microstructure. Over time, the sphere gradually grows inside the cell domain and pushes a finite volume of fluid out of the cell domain during the clogging stage. The cell's initial porosity and macroscale permeability of the depth filter then reduce gradually over time. Most recently, Printsypar et al. (2018) studied the effects of varying microstructure on the depth filter's

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removal performance and effective homogenized parameters such as permeability, porosity etc., for different filtration scenarios such as constant-flux and constant-pressure flow cases. The authors then made recommendations for the range of operating parameters which can improve an arbitrary filter's filtration performance under the different flow conditions (constant-flux or constant-pressure).

The above-discussed analytical contributions to model depth filter's clogging behavior are useful towards the engineering designs of new filters. However, extending their analysis to model the specific clogging conditions for the predictive maintenance objective has not been done by far. For example, uncertainties remain for the possibility of leveraging the authors' proposed models to quantify the complex adsorption-desorption processes in adsorbers (depth filters) as there were no considerations for the desorption phase in their original derivations. In addition, the engineering predictions made by those models have not yet been verified with real-world measured data which is necessary to confirm the models' predictive accuracy for on-field applications. Printsypar et al. (2018) too mentioned that it is still not possible for their present model to estimate complex filter parameters such as reaction rate coefficient during the clogging stage.

Other insightful contributions which modelled the complex clogging problem in depth filters were also made by Ray et al. (2012) and Royer (2018). The former work analysed the transient variations to the periodic microstructure during the trapping of colloids in porous media system which is, to an extent, close to the recent work by Printsypar et al. (2018). The authors, however, focused on the complex interplay between attachment and detachment mechanisms, colloidal interaction forces and a changing microstructure in terms of its dimensions. Their models can provide useful quantitative understanding of effects of those processes on pore clogging and porosity changes over time. Finally, the work of Royer (2018) elegantly derived the homogenized representations, till much higher orders which can be computationally difficult, to model the advection-diffusion mechanism in porous media systems. The author's work is again a must-read for readers interested to extensively learn about harnessing the analytical technique for other suitable field applications. Again, however, the models deriving from the above-mentioned research works (as

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summarized in Table 2.1.1) have not been verified with real-world measured data for predictive verifications.

In this thesis study, the depth filter is first modelled as a random configuration of collector spheres, as representation of the porous media grains, under creeping flow conditions whereby the microscale filtration Reynolds number is very much smaller than unity as mentioned. The proposed homogenization theory coupled with the multiscale perturbation analysis is then leveraged to model the different clogging condition in depth filters. For physical clogging, the assumed trapping stage over time results in larger collector spheres which reduce the periodic cell's porosity under creeping flow conditions. At the same time, the macroscale filter's average permeability reduces over time which encapsulates the clogging behavior. Importantly, an arbitrary initial arrangement of the media grains is adopted for the periodic cell domain which differ from previous studies (Battiato and Tartakovsky, 2011; Bruna and Chapman, 2015; Dalwadi et al., 2015, 2016; Korneev and Battiato; 2016) before applying the homogenization step with the perturbation analysis at the varying scales (microscale to macroscale). Importantly, the present analysis ensures a much smaller pore-scale separation among the spheres than that of the periodic cell domain to maintain a disordered arrangement of the collector spheres within the same cell domain (to be further explained in Chapter 3). This scenario is realistic as the analysis only regards fully saturated flow conditions inside real-world depth filters. Measured data (after appropriate data augmentation) is then adopted to perform supervised learning with the derived homogenized representation for quantifying the physical clogging behavior inside the depth filter and builds towards the predictive maintenance objective.

The major difference from previous notable research works (Battiato and Tartakovsky, 2011; Bruna and Chapman, 2015; Dalwadi et al., 2015, 2016; Korneev and Battiato; 2016) is that the present analysis avoids solving for the homogenized parameters (permeability, diffusion coefficient etc.) via exact computations or numerical approximations. Usually, the latter requires the user to adopt an idealized packing configuration in the cell domain that may not emulate real-world depth filters of complex packing. For random media packing, the zig-zap effect has been confirmed

Table 2.1.1. High-level description of key modelling works which leverage on homogenization theory with multiscale perturbation analysis to model fluid and mass transport characteristics, and clogging problems in porous media systems

Authors & publication years	Contributions	Shortcomings
Mei et al. (1996); Mei and Vernescu (2012a); Mei and Vernescu (2012b)	<ul style="list-style-type: none">• First few researchers who rigorously derived analytical functions, via the homogenization theory with multiscale perturbation analysis, to analyse complex fluid and mass transport problems in porous media domains	<ul style="list-style-type: none">• Validity of approach has not been tested on measured data for engineering predictions
Dalwadi et al. (2015); (Dalwadi et al., 2016); Printsypar et al. (2018)	<ul style="list-style-type: none">• First few researchers who leveraged on the same hybrid technique to model the clogging/trapping dynamics in depth filters	<ul style="list-style-type: none">• Validity of approach has not been tested on measured data for engineering predictions• No considerations for detachment processes when modelling the clogging stage
Battiato and Tartakovsky, (2011); Korneev and Battiato; (2016); Battiato et al. (2019)	<ul style="list-style-type: none">• First few researchers who rigorously derived analytical functions, via the homogenization theory with multiscale perturbation analysis, to analyse complex fluid and mass transport problems in porous media domains	<ul style="list-style-type: none">• Validity of approach has not been tested on measured data for engineering predictions

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to be significant (Long and Hilpert, 2009; Montessori et al., 2016) in affecting the diffusion mechanism. By far, there have been several quantitative representations available to estimate the complex diffusion coefficient for depth filters with simplified settings (Yao et al., 1971; McDowell-Boyer et al., 1986). However, there is currently no generic quantitative expression to pre-estimate the diffusion coefficient, which depends on the contaminant size, concentration, fluid temperature etc. and can vary substantially among different porous media scenarios/configurations. Quantifications of this complex diffusion parameter is particularly important in porous media systems undergoing creeping flow conditions. Hence, the present analysis encapsulates the complexity of the diffusion coefficient by adopting measured data to perform supervised learning of the key parameters derived from the homogenized representations for the respective clogging analysis. Appropriate estimations of the diffusion coefficient and other complex filter parameters such as reaction rate coefficients can then be performed via the supervised learning step.

Unlike from the physical clogging analysis, no transient variations to the collectors' diameters will be considered for the chemical clogging behavior. Instead, the surface concentration of contaminants at the collector spheres is taken to increase gradually over time due to the diffusive transport and subsequent net adsorption (adsorption rate greater than desorption rate) of the concerned contaminants from the fluid phase onto the impermeable surfaces. At a certain stage, a complex close balance between the surface and fluid concentrations is attained, i.e. near-equilibrium concentration state, which also involves the desorption flux of the initially adsorbed contaminants from the collectors' surfaces (Feder and Giaever, 1980; Johnson and Elimelech, 1995) back into the fluid phase. The homogenized representation derived then contains a unique parameter to quantify the near-equilibrium concentration state whereby both adsorption and desorption processes are concurrently materializing inside the adsorber as building towards its exhaustion stage. Different groups of measured data are then used to train the unique parameter, followed by testing the model's predictive capability to achieve the outlined objective. Note that there have been no attempts by far in using the proposed analytical approach to model the chemical clogging conditions in depth filters caused by the concurrent adsorption-desorption processes taking place.

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Finally, modelling the biological clogging condition in depth filters involves the combination of the above-mentioned settings from the physical and chemical clogging analyses respectively. The transient growth of the collector spheres inside the periodic cell domain is due to the dynamic development rate of a thin biofilm matrix around the spheres caused by the biological absorption of the concerned contaminants over time. The key engineering physics lies with quantifying the complex reaction processes within the thin biofilm layer which depends on a specific timescale based on appropriate physical arguments. At the same time, to account for the exhaustion phase of the media grains inside biological activated filters (biofilters) as discussed, the proposed model considers the absorption/desorption behavior of the contaminants at the interphase between the sphere's surface and biofilm matrix as building towards the exhaustion stage of the biofilter. Measured data from biofiltration column experiments is then adopted to calibrate the proposed model with a reduced feature space to verify its predictive accuracy for the predictive maintenance objective. Again, this approach has not been attempted before in the literature by far.

2.2. Physical clogging analysis in depth filters

Iwasaki (1937) and Mints (1966) were several of the pioneers to highlight the usefulness of the depth filtration process for purification purposes. Ives (1970) extensively discussed on the different particle removal mechanisms (interception, straining, gravitational sedimentation, inertial impaction, etc.) involved during rapid filtration, built upon the earlier works of Ison and Ives (1968), to quantify depth filter's purification performance over time. The notable Yao's filtration model (Yao and O' Melia, 1968; Yao et al., 1971) was subsequently built to model the particle transport along the fluid streamlines around a singular collector sphere and their subsequent attachment, via sedimentation, interception and Brownian diffusion, at the impermeable surface of the sphere. One notable limitation of their analysis was the omission of the periodic flow conditions around the singular sphere to account for the effects of neighbouring grains on the filter's performance. Hence, the proposed Yao's model (Yao et al., 1971; MWH, 2005) to quantify depth filters' removal efficacy may not emulate the conditions of real-world filters entirely. Another notable modelling study was by Adin and Rebhun (1977) which quantified the particle detachment

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mechanism in depth filters by considering the fluid momentum and mass continuity equations for engineering predictions of the filter's breakthrough time. O'Melia and Ali (1978, 1979) then further modified the Yao's model to approximate the energy loss rate occurring during clogging conditions, by assuming that the trapped particles serve as additional collectors to improve the filter's performance over time.

O'Melia and Ali model (1978, 1979) was later modified by many researchers to quantify the particle size effect on the filter's energy loss rate during effective clogging stage. Mackie and Bai (1991) modelled the particle size distribution on the filter's changing effluent concentration and head loss during its physical clogging stage. The authors concluded that assuming a mean particle size in the influent suspension was insufficient to accurately compute the filter's head loss over time. However, using a singular parameter to quantify a range of particle size remains difficult till today. Darby et al. (1992) too confirmed that using an average particle size for model calibration did not perform as well as that when adhering to a defined particle size distribution in predicting the filter's head loss during its physical clogging stage. Boller and Kavanaugh (1992) modelled the effects of particulate size, density, filtration rate, and media sizes on the filter's head loss development rate during effective clogging. Tobiason and Vigneswaran (1994) modified the original model of O'Melia and Ali (1978, 1979) by using a surface area based linear model to account for the particle size effect on the filter's head loss incurred over time. The effects of using varying types of coagulants on the head loss was also considered in the authors' model development process. Veerapaneni et al. (1993, 1997) and Wiesner (1999) extensively studied the particle size on the filter's head loss development rate and confirmed that smaller particles resulted in higher head loss over time due to the larger surface area effects exerted via their close compaction with the media grains during the physical clogging stage. The effect becomes vice versa for the trapping of bigger particles inside the filter. In the later chapters, the present analysis by the proposed DRFM model will capture the unique particle size effect on the filter's performance and head loss development rate.

Another notable work was by Mays and Hunt (2005, 2007) which modified O'Melia and Ali model (1978, 1979) and adopted 43 previous sets of filtration sets from a lab-

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scale depth filter setup to model the filter's head loss development rate due to physical clogging of specific contaminants. Their studies extensively examined the hydrodynamic and chemical effects on the clogging behavior. For example, the authors demonstrated that slower superficial velocity into the filter improves the filter's removal performance over time and fully destabilized suspensions can also achieve the same performance objective. Their resulting model predicted the filter's energy loss due to clogging by montmorillonite. Experimental investigations of the filter's media size, hydraulic loading rate, particle concentration etc., have also been carried out to model their respective effects on filter's performance and head loss development rate during the physical clogging stage (Kau and Lawler, 1995; Stevenson, 1997; Williams et al., 2007; Han et al., 2009; Kim and Lawler., 2012; Bennacer et al., 2013; Alem et al., 2015). It is worth noting that the above-discussed studies only analysed the filtration of low turbid influents, likewise in an early research study (Ives and Pienvichitr, 1965), and their suitability for modelling the effects of filtering high-turbid influents on an arbitrary filter's head loss development rate has not been verified extensively by far. In addition, there have been limited effective predictive models which can pre-estimate depth filter's breakthrough time, due to the effective physical clogging stage, by using known operating parameters a priori.

Computational methods have since been advanced to simulate the physical clogging behaviour in emulated depth filter configurations. One example was the use of the commercially available FLUENT computational fluid dynamic (CFD) software by Tung et al. (2004) to study varying packing configurations on the physical trapping of suspended solids of different sizes under a wide combination of physical forces such as gravity, hydraulic drag, etc. Their simulation results indicated that face-centered packing configuration in depth filters resulted in the highest trapping efficacy over time, but also the largest pressure drop in terms of the head loss computations. Furthermore, the authors' results suggested that body-centered packing resulted in the best removal performance when compared to relevant experimental data. Hassan et al. (2013) also adopted FLUENT to simulate the trapping of varying concentrations (steady-state and sudden spikes) of nanoparticles (NP) in saturated sand filters. Their simulation results indicated that sudden spikes in NP concentrations can be effectively removed inside the emulated sand filters. Till today, however, the challenge of

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simulating the physical (and other types) clogging condition in emulated depth filters involves the modeller to effectively account for the complex meshing of the many collector grains and their inherent pore structures. This remains a huge computational challenge.

To address the above-described numerical challenge, researchers have since proposed different computational methodologies. Examples include using graphic processing units (GPUs) to couple both CFD with discrete element method (DEM) to simulate 25 million of particles in fluidized granular system (Jajcevic et al., 2013) which simulation results agreed well with experimental data from Van Buijtenen et al. (2013). Muljadi et al. (2015) examined non-Darcy flow conditions via pore-scale simulations of complex three-dimensional (3D) X-ray images and proposed alternative non-Darcy coefficient for the different simulated samples and compared with respective experiments. The above-mentioned techniques, however, require niche computing expertise which may not be easily made available to field engineers.

Lattice Boltzmann Method (LBM) has also been adopted to simulate the filter's physical clogging dynamics. Long and Hilpert (2009) leveraged on LBM to develop a new correlation for the diffusion mechanism to quantify depth filter's removal efficacy of both small and large particles. Their model can be useful to the design of new depth filters for performance optimization during operations. Abdelhamid and El Shamy (2016) simulated the transient pore-scale migration of base-soil particles through depth filters of varying media sizes. Generally, the simulation results for the trapping behavior (erosions in their case study) agreed well with respective measurements which can again be helpful for the engineering design of new depth filters. Other conventional numerical techniques have also been used to simulate the physical clogging behavior in filters. For example, Ojha et al. (2011) adopted finite difference methods to discretize the mass continuity and kinetic equations to model the filter's performance over time and space for engineering predictions. Assumaning et al. (2012) applied the forward-time-central-space (FTCS) method together with Kalman filter technique and its variants to model groundwater contaminant based on a 3D subsurface advection-dispersion-reaction model. The authors reported a 70% reduction in the error deviation between the model's predictions with measured values.

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Notwithstanding the computational novelty of the above-discussed numerical studies, it is worth noting that those models are still not likely to perform the predictive maintenance act for arbitrary depth filters, based on known physical parameters a priori, undergoing the physical clogging condition over time. In summary, while computational tools are useful to provide us with quantitative understanding of the filter's complex physical clogging behavior, the resulting computational cost remains difficult for field engineers to efficiently perform large variations to the filter-related parameters. The required computational cost and niche expertise for very accurate engineering predictions may also hinder industrial applicability on a large-scale.

2.3. Chemical clogging analysis in depth filters

As discussed, chemical clogging is caused by the precipitation of contaminants from the fluid phase within the depth filter and their subsequent adsorption onto the surfaces of the media grains by overcoming the hydrodynamic, electrostatic and van der Waals' forces between the contaminants and sphere's surface. Such clogging usually takes place after long periods of creeping flow filtration conditions inside the filter (Jeong et al., 2018). The present analysis models the concurrent adsorption and desorption processes of contaminants taking place inside depth filters which will be discussed in greater detail in Chapters 3 and 4 subsequently. During the initial operational phase, the adsorption rate outweighs the desorption rate significantly due to the relatively clean state of the media grains. Over time, as adsorption of contaminants takes place at the impermeable surfaces of the grains, the surface concentration of contaminants increases which leads to a reducing concentration gradient between the grain surface and the neighbouring fluid domain. Consequently, the desorption flux of contaminants from the grain surfaces back into the fluid phase becomes increasingly important which contribute to the desorption mechanism. On a whole, there will still be a net adsorption (adsorption rate greater than desorption rate) process taking place in the depth filter as long as the effluent concentration of contaminants is less than that of the influent feed in average values. For simplicity, filter systems undergoing a net adsorption mechanism, i.e. adsorption rate greater than desorption rate, can be defined as adsorbers whereby exhaustion of their deployed media occurs when the adsorbers' effluent concentration of contaminants exceeds a pre-defined threshold

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value. Subsequently, the deployed media must subsequently be reactivated (Martin and Ng, 1984; San Miguel et al., 2001; Benstoem et al., 2017) via appropriate treatment processes for redeployment into the adsorber.

The significance of the complex adsorption-desorption mechanisms taking place inside adsorbers has been verified by previous studies which investigated the effects of the coupled process on different types of contaminants (Rumynin et al., 2005; Mishra et al., 2013; Kyzas et al., 2013; Mishra, 2014; Rani and Sud., 2015) in batch or column experimentations. Rumynin et al. (2005) modelled the adsorption-desorption processes of radionuclides solutions via experimental means. The authors reported that the initial effective adsorption of radionuclides was eventually affected by the concurrent rise in the corresponding concentrations within the porous media system of sedimentary rocks. Their empirical observations aligned with the above-discussed statement regarding the adsorption and desorption processes taking place simultaneously during operations and how both reactions rates change respectively. Mishra et al. (2013) analyzed the force field for tricalcium silicate, which is an important constituent for cement, and its subsequent impact on the adsorption of organic molecules from the nanoscale perspective. The authors reported that the adsorption process reduced the surface forces which then affected the measured grinding efficiencies. Kyzas et al. (2013) too confirmed a lack of analytical modelling studies for the desorption mechanism. The authors then modelled the batch adsorption-desorption of dyes and reported that the total solute mass, i.e. concentration, conservation principle was likely to be responsible for the decline in adsorption efficacy during their experiments. Again, this observation aligned with the above hypothesis regarding the adsorption-desorption processes.

Mishra (2014) instead demonstrated that the specific type of adsorbates, i.e. the contaminants to be adsorbed, affected the desorption observations in their experiments. Rani and Sud (2015) reported that increasing media (soil) temperature reduces the adsorption rate of pesticides and increases the rate of desorption of the initially adsorbed contaminants from the soil surfaces. Their results will be useful for the operating design of adsorbers removing pesticides in intake feedwater. In summary, the delineated information of those previous experimental/modelling studies confirm that the present analysis must effectively model the complex adsorption-

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desorption processes materialising inside porous media systems, in order to quantify their impact on the timing for an arbitrary adsorber to reach its respective exhaustion stage based on known operating parameters a priori.

Benstoem et al. (2017) specifically identified the following parameters to establish any adsorber's breakthrough curve till its exhaustion stage is reached: (a) influent's contaminant concentration, (b) empty bed contact time (EBCT), (c) type of material, (d) backwashing procedures, (e) amount of suspended solids, and (f) energy loss inside the adsorber. For generality, the breakthrough profile of a typical adsorber, which undergoes both the adsorption and desorption processes concurrently during operations, can be schematically described in Figure 1 as evident in several previous studies (Smith.,1994; Velten et al., 2011; Treumann et al., 2014; Zhao et al., 2016; Zietzschmann et al., 2016) for removing ammonium ions, colloids, micropollutants and natural organic matters in column tests.

Figure 2.3.1. Illustration of proposed phase-1 and phase-2 concentration profiles in operating seepage filters, undergoing net adsorption mechanism, as building towards their exhaustion stages.

From Figure 2.3.1, the characteristic effluent concentration profile of an operating adsorber, prior to its exhaustion stage, can be divided into two key phases, namely: (a) phase-1 stage whereby there is a consistent rise in its effluent concentration over a short period of time; and (b) phase-2 stage whereby the effluent's concentration gradient over time approaches a quasi-steady-state condition over a long period of time as building towards the adsorber's exhaustion stage. As discussed, there has been limited engineering models available which can model both phase-1 and phase-

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2 stages of an operating adsorber for contributing to its predictive maintenance act based on the exhaustion stage criteria and known operating parameters.

To derive the characteristic concentration transient profile (plots normalized effluent concentration against filter's throughput units) in Figure 2.3.1, Smith (1994) proposed a defined multicomponent model incorporating ideal adsorbed solution theory (IAST) to analyse the adsorption behavior of natural organic matters (NOMs) in lake water. The author's model was able to quantify the effects of varying influent concentration on the timing for a dynamic fixed-bed model to reach its exhaustion stage. Velten et al. (2011) deployed two pilot-scale granular activated carbon (GAC) adsorbers to again examine the adsorption behavior of NOMs from lake water as the influent feed into both filters. The characteristic profile of Figure 2.3.1 was observed by the authors when removing humic materials, building blocks and low molecular weight (LMW) organics. They too reported that the internal surface area of the GAC media greatly affected the varying weight groups of organics whereby the removal efficacy within the adsorber increased with a reducing size of NOMs. Treumann et al. (2014) confirmed that only adsorption column tests can result in the characteristic profile of Figure 2.3.1 as irreversible adsorption (attachment) process took place in their batch experiments. In addition, they reported that the differing hydrodynamic forces between the batch and column tests resulted in dissimilar rates of adsorption over time. Based on our own experiences, that observation is most likely due to major differences in the grain-to-column diameter ratio of both settings which affect the contaminant movement along the fluid streamlines and shearing forces acting upon the media grains.

Zhao et al. (2014) examined the adsorption behavior of complex ammonium ions in both batch and column tests, whereby the latter component resulted in the characteristic concentration profile in Figure 2.3.1. The authors too demonstrated that increasing temperatures reduced the adsorption capacity of the concerned ions on the media grains while variations in the Darcy flow velocity had minimum effect on the adsorption behavior. Finally, Zietzschmann et al. (2015) studied the removal of organic micro-pollutants (OMPs) from water and wastewater treatment plants using small-scale GAC tests. They then recommended that field engineers must know the

concentrations of the influent OMPs and LMW organics for any given settings in order to leverage on their empirical models to predict the breakthrough and exhaustion stages of GAC media when treating other waters. In summary, the above-discussed research works indicated that experimental/empirical analysis has been the main driver to build the scientific community's present knowledge relating to modelling the chemical clogging condition in depth filters caused by the adsorption-desorption processes. However, there have still been limited computational and/or analytical analyses of the adsorption-desorption processes by far which hinder the development of generic predictive models for the predictive maintenance act of depth filters undergoing the chemical clogging behavior over time.

2.4. Biological clogging analysis in depth filters

For depth filters to undergo biological clogging condition over significant long periods, porous media such as activated carbon is most suitable for deployment due to their large BET surface area, i.e. high surface-area-to-volume ratio, and high adsorptive capabilities, as in the case for the chemical clogging scenario from the preceding section. This unique physical characteristic enhances the complex attachment rate of microbes/contaminants from the fluid phase to the surface matrix of the media grains (MWH, 2005; Granger et al., 2016). Till date, there have been significant number of experimental studies which adopted granular activated carbon (GAC) materials to investigate the complex biofiltration mechanism (Rhim and Yoon, 2007; Hoang et al., 2008; Yapsakli and Cecen., 2010). For example, Rhim and Yoon (2007) developed a plug-flow stationary solid-phase column model which modelled the breakthrough profile of dissolved organic carbon (DOC) in a biological activated carbon (BAC) pilot plant. The authors reported that the measured breakthrough value for DOC in the investigated pilot plant approximated to 0.425 under the throughput bed volumes of 10,000, which was close to the predicted breakthrough value of 0.45 by their proposed model. Their results confirm that it is possible for computational modellers to develop engineering tools which can encapsulate the complexity of the biofiltration mechanism as tailored to specific operational conditions.

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Hoang et al. (2008) investigated the effects of varying media depths, influent concentrations, filtration rates and backwashing mechanisms on biofilters' performance over time for removing organic matter from seawater. The authors concluded that daily filter maintenance via backwashing, for mitigating its physical clogging condition, did not affect the system's organic removal performance due to minimum flushing of the residing microbes from the operating filter. At the same time, they reported that the biofilter performed best when treating lower influent concentrations at lower hydraulic loading rates. Yapsakli and Cecen (2010) investigated the effects of varying types of GAC materials, namely, steam activated and chemically activated ones, on the biodegradation of DOC in BAC columns over time. The authors confirmed that steam activated carbon materials enhanced the biodegradation efficacy of DOC in BAC columns and reported that the biodegradation process can generally extended the operational lifespan of BAC filters, hence delaying their breakthrough phase. Their finding can thus be useful to identify the biofilter's breakthrough criteria of either: (a) exceedance in the effluent concentration profile at a certain throughput unit; or (b) approaching the limiting permeability value over a significant throughput period, for future model development. Previous studies have also reported that the biofilter's empty bed contact time (EBCT), i.e. residence time, significantly affects the system's removal performance over time whereby longer EBCTs lead to higher removal efficacy of specific contaminants (Liao et al., 2013).

In general, the biological clogging behavior in depth filters can be quantified by the type of biological activity taking place between two states (Zhang, 2017), namely: (a) microbes which exist in planktonic state; and (b) microbes which exist inside a complex extracellular polymeric matrix, i.e. biofilm layer around the media grains. The focus is to propose alternative engineering approaches which can model the complex biofilm layer in real-world biofilters for the predictive maintenance objective. Biofilms generally protect bacteria communities/colonies from the fluid shearing effect and binds them to rigid media surfaces having large BET surface area (Chang and Rittmann., 1987a) as stated earlier. To achieve the desired operational condition, biofilters require significant amount of residence time (EBCTs) together with the right nutrient balance for the biofilm development over time (Granger et al., 2016). If the conditions are non-existent, the residing microbes are likely to exist in planktonic state inside the fluid

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phase of the biofilter system which may not contribute significantly to the filter's performance over time.

Traditionally, mathematical modelling of the complex processes taking place inside biofilters require computational modellers to leverage on representations which quantify the following components: (a) substrate mass transport behavior; (b) diffusion of substrate in the liquid phase of the porous media system; (c) complex biofilm development inside the filter over time; and (d) concurrent adsorption and utilisation kinetics of the substrate (Chang and Rittmann., 1987a; Kim, 1994; Chaudhary et al., 2003; Shim et al., 2004). Chang and Rittmann (1987a) was one of the few pioneers to model the complex biofilm behavior by including the diffusion effects inside the biofilm via Fick's law together with non-linear reaction processes taking place. In addition, their mathematical model assumed a first-order biofilm loss with respect to the mass of biofilm available around the media grains and adopted the Freundlich isotherm to quantify the adsorption process occurring concurrently. The authors then adopted numerical finite difference methods to resolve the complex mathematical model for engineering predictions. Their work continues to be notable as the proposed model accounted for many empirical representations to effectively encapsulate the complexity of biofilm development in biofilters. Hence, with availability of real-world experimental data, it becomes possible to calibrate the empirical coefficients via numerical iterations. In their later paper (Chang and Rittmann., 1987b), the authors verified their proposed model by using experimental data derived from a lab-scale column reactor system, together with appropriate assumptions made to various parameters. In total, 12 unique coefficients were calibrated with the measured data to approximate the substrate concentration inside the column system over time which agreed well with the respective data. The authors also concluded that the adsorption mechanism was generally less significant than the biodegradation process in removing the available substrate from the intake feed, which can be a useful assumption or finding for new model developments to quantify the complex biofiltration process.

Kim (1994) adopted similar mathematical methodology as that of Chang and Rittmann (1987a) via the following means: (a) adhering to the Freundlich isotherm to model the adsorption process; and (b) modelled the biological parameters via the

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traditional Monod kinetic representation. For model calibration, the authors instead examined the biofiltration of glucose and sucrose as the target substrate, which are generally readily biodegradable, inside column tests. In addition, the authors compared the operational effectiveness between biological-activated and non-biological-activated columns to again demonstrate the limited impacts of adsorption and the enhanced effects of biodegradation in terms of the biofilter's removal performance over time. It was concluded that adsorption affected the initial removal, while biodegradation controlled the filter's steady-state performance over long periods. Likewise, their results can provide useful starting assumptions for new model developments for quantifying the complex biofiltration mechanism and will thus be adopted in this thesis study as quantitatively described in the later section.

The derived experimental data of Chang and Rittmann (1987b) was also undertaken by the research work of Shim et al. (2004) to model the removal performance of biofilters. Instead of adhering to available empirical representations to quantify the complex microbial behavior, the authors developed the predictive model based on the biofilter's operating condition and influent characteristics. The Sips isotherm was leveraged to quantify the adsorption process taking place, which was again justified by the authors to have minimum contributions to the biofilter's effective removal efficacy over time. The transient reduction in the available specific surface area of the GAC media for biofilm development then attributed to the gradual reduction in the biofilter's removal performance. In another study by Yapsakli and Cecen (2010), the authors instead reported a steady-state removal performance by the biofilter, for removing organic matter from surface water collected from reservoir, following the exhaustion of the available GAC media inside the biofilter, i.e. adsorption effects become insignificant. Similar trend was also recently reported by the research work of Korotta-Gamage and Sadasivan (2017) for removing organic carbon from surface waters. In summary, previous studies have justified the dominance of the biodegradation effect over the adsorption mechanism, of which the latter is mainly responsible for the chemical clogging condition as extensively discussed previously, for the effective removal performance of biofilters over time.

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While the contributions by previous research studies are insightful and important, it is worth noting there have been limited or no generic engineering models available which can be tailored to any variations in the operational conditions (media depths, types of contaminants removed, hydraulic loading rates, etc.) of real-world biofilters for the predictive maintenance objective. In addition, significant number of empirical representations (Monod's kinetic representation, etc.) are usually involved for engineering predictions which again restrict extending the final model's predictive capability for any varied set of operational conditions. To address this limitation, future research studies should focus on leveraging first principle representations, which quantify the flow and mass transport problems in porous media systems, as slowly building towards a general engineering model to fulfil the following criteria: (a) minimize the number of empirical representations; and (b) perform the predictive maintenance act for operating biofilters based on any arbitrary set of operational conditions and data availability.

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Chapter Overview:

This chapter systematically describes the first principle equations adopted to quantify the creeping fluid flow condition and mass transport of contaminants in the pore-spaces of porous media systems, having complex packing geometry, which undergo physical and chemical clogging conditions over time. The governing equations then undergo normalization procedures with respect to suitable mass, spatial and time scalings which are characteristics of the specific clogging behavior being modelled. Homogenization of the normalized equations is then performed by using the multiscale perturbation analysis, which leverages on a sufficiently small perturbation parameter defined a priori, to derive varying homogenized averaged representations for modelling the different types of clogging behavior over space and time.

Sections 3.1 and 3.2 describe in quantitative details for the first principle equations and the normalization steps, respectively, adopted to model the transient physical and chemical clogging behavior taking place inside porous media systems. Following which, Sections 3.3 and 3.4 derive the respective homogenized averaged representations to quantify the specific type of clogging condition being modelled over space and time.

3.1. Model Development

3.1.1. First principle equations

Generally, porous media grains are packed randomly inside a macroscale depth filter which complicates the fluid dynamics and mass transport behavior of contaminants inside the filter's global pore spaces. To reduce the complexity of the slow filtration (creeping flow) problem responsible for the physical, chemical and biological clogging conditions taking place inside the filter, we first model the macroscale system as a network of randomly arranged three-dimensional (3D) rigid collector spheres which emulate the deployed media grains. A periodic microstructure is then assumed (Figure 3.1.1), as extracted from the global network, to randomly pack several ideal spheres inside a 3D box having the length scale of $O(l)$ whereby l is the characteristic average size of each media grain and is very much smaller than the characteristic macroscale

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media depth of L . A very small perturbation parameter, defined as $\varepsilon = \frac{o(l)}{o(L)}$, will then be leveraged in the subsequent sections to perform the multiscale perturbation analysis for deriving the macroscale quantities in all clogging scenarios (physical, chemical and biological conditions).

Figure 3.1.1. Simplified representation of disordered microscale packing geometry of media grains (represented by collector spheres) for seepage filters.

To maintain a disordered arrangement of the spheres in each periodic cell domain, the average pore-scale separation between the spheres (μ) must be much smaller than l (Davit et al., 2013; Chew and Law., 2019a, 2019b) as shown in Figure 3.1.1. This assumption is true for real-world depth filters as the grains are usually compacted randomly under fully saturated conditions. We emphasize that the current arrangement of the collector spheres in Figure 3.1.1 is only arbitrary, i.e. random, and there can be many different combinations of arranging the spheres in each cell domain. However, regardless of the arrangement choice for the media grains within each cell domain, the pore-scale fluid properties (pressure, velocity and concentration) are assumed to be spatially periodic from cell to cell while varying slowly over L .

Within each periodic cell domain (Figure 3.1.1), the solid sphere is defined as $\Omega_s \subset \mathbb{R}^3$ while the fluid phase is defined $\Omega_f \subset \mathbb{R}^3$. The interface between the solid and fluid phases is taken as $\Omega_{fs} \subset \mathbb{R}^3$. Coupling both phases then results in the whole periodic cell domain defined as $\Omega \subset \mathbb{R}^3$. The fluid motion at low microscale Reynolds numbers (much smaller than the value of unity) in the pore space of each cell domain

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is governed by the incompressible steady state Stokes equation in (3.1.1) and the mass continuity equation in (3.1.2).

$$\frac{\partial u_i^*}{\partial t^*} = -\frac{\partial p^*}{\partial x_i^*} + \frac{\partial}{\partial x_j^*} \left(\nu \frac{\partial u_i^*}{\partial x_j^*} \right), \quad x^* \in \Omega_f \quad (3.1.1)$$

$$\frac{\partial u_i^*}{\partial x_i^*} = 0, \quad x^* \in \Omega_f \quad (3.1.2)$$

where x^* is the position vector, u^* the velocity vector, ν the fluid kinematic viscosity, p^* the fluid pressure, and t^* the time.

For each modelled clogging condition (physical, chemical and biological), the concerned contaminants being removed in the depth filters are initially transported, via advection and diffusion, inside the fluid phase of each periodic cell domain which is quantitatively described as:

$$\frac{\partial c^*}{\partial t^*} + \frac{\partial (c^* u_i^*)}{\partial x_i^*} = \frac{\partial}{\partial x_i^*} \cdot \left(D_p^* \frac{\partial c^*}{\partial x_i^*} \right), \quad x^* \in \Omega_f \quad (3.1.3)$$

whereby the concentration, c^* is the mass of contaminants per unit volume of fluid, and D_p^* represents an unknown coefficient responsible for the complex diffusion of the concerned contaminants inside the random porous matrix. We note that this diffusion coefficient will vary among the different types of contaminants, which contribute to the varying type of clogging condition taking place inside the filter, due to differing operating parameters such as particle size, temperature, concentration, etc.

Generally, the diffusion process is expected to be strongly associated with the different clogging scenarios taking place inside the depth filters due to the creeping flow condition, as quantified by (3.1.1), whereby the microscale Reynolds number is very much smaller than the value of unity as mentioned. At the same time, the microscale Peclet number will also be very small due to the very small velocity scale. A very small microscale Peclet number indicates that the diffusion process will dominate the advection process for the contaminants' transport inside the pore spaces (fluid phase) of each periodic cell domain.

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In terms of interfacial mass transport in each clogging scenario, we assume that the concerned contaminants undergo an assumed independent first-order removal and detachment processes at the sphere's boundary (S^*), as defined in (3.1.4).

$$-\frac{\frac{\partial S^*}{\partial x_i^*}}{|\nabla S^*|} \cdot \left(D_p^* \frac{\partial c^*}{\partial x_i^*} \right) = k_{rem} c^* - k_{det} c_s^*, \quad x^* \in \Omega_{fs} \quad (3.1.4)$$

where S^* is the boundary of the collector sphere with $\frac{\partial S^*}{\partial x_i^*}$ being its outward normal vector acting from the boundary, k_{rem} and k_{det} are the respective unknown removal and detachment rates of the concerned contaminants having the dimensions of $[LT^{-1}]$, and c_s^* the average concentration of removed contaminants from the fluid phase at the spheres' boundaries along the media depth.

Note that k_{rem} and k_{det} can vary over time due to the following conditions: (a) the changing surface concentration of removed contaminants from the fluid phase around the collector spheres; and (b) the changing bulk fluid concentration of the same contaminants inside the pore-spaces of the periodic cell domain during clogging. We emphasize that the linear relationship in (3.1.4) is only an assumption to facilitate the analytical derivations, which then build the basis for us to adopt measured data to model the filter's clogging complexity via supervised learning. Note that a generic model is currently being proposed which can be tailored to any specific types of contaminants being removed in depth filters undergoing the different clogging conditions, whereby the unknown removal and detachment coefficients can subsequently be calibrated via supervised learning with measured dataset.

Within each cell domain, the no-slip flow condition is also imposed at the spheres' boundaries in each cell domain for each clogging scenario, defined as:

$$u_i^* = 0, \quad x^* \in \Omega_{fs} \quad (3.1.5)$$

Note that (3.1.1 – 3.1.5) quantify the general creeping fluid flow condition and mass transport physics in depth filters, regardless of the specific type of clogging behavior being modelled. In the following sub-sections, the exact reaction mechanism at the

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spheres' boundaries responsible for each specific clogging condition is described in quantitative details.

3.1.2. Mechanics responsible for physical clogging condition

Physical clogging condition in depth filters, under creeping flow condition, is caused by the trapping of turbidity particles over long periods of operations as discussed earlier. This phenomenon is quantified by the transient growth of collector spheres (d^*) along the macroscale media depth which results in an ever-changing outward normal velocity acting at the boundary of each growing sphere as follows:

$$-\frac{\frac{\partial S^*}{\partial x_i^*}}{|\nabla S^*|} \left(\frac{\partial d^*}{\partial t^*} \right) = u_i^*, \quad x^* \in \Omega_{fs} \quad (3.1.6)$$

The growth of the sphere's initial diameter along the media depth is coupled with the accumulation of turbidity particles around the sphere's boundary by the following volume conservation principle:

$$\frac{\partial d^*}{\partial t^*} = -\frac{1}{\rho_p} \frac{\frac{\partial S^*}{\partial x_i^*}}{|\nabla S^*|} \cdot \left(D_p^* \frac{\partial c^*}{\partial x_i^*} \right), \quad x^* \in \Omega_{fs} \quad (3.1.7)$$

where ρ_p is the bulk density of the deposits of turbidity particles.

Effective clogging stage is typically observed during the physical trapping of turbidity particles which concurrently leads to a gradual reduction in the depth filter's global permeability over time. Hence, k_{det} is taken to be negligible in (3.1.4) to model the physical clogging condition in depth filters in the later homogenization procedures.

3.1.3. Mechanics responsible for chemical clogging condition

As explained earlier, chemical clogging condition in depth filters is caused by the net removal process (removal rate greater detachment rate), i.e. net adsorption process, of precipitated contaminants, from the fluid phase, at the spheres' boundaries over long periods of operations. Note that the removal (k_{rem}) and detachment (k_{det}) rates now represent the adsorption (k_{ads}) and desorption (k_{des}) processes respectively for

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modelling the chemical clogging condition in depth filters. For convenience, filters which undergo the net adsorption process over time can be termed as adsorbers.

As discussed in Section 2.3, a typical effluent concentration profile (Smith.,1994; Velten et al., 2011; Treumann et al., 2014; Zhao et al., 2016; Zietzschmann et al., 2016) of an operating adsorber is represented in Figure 2.3.1, whereby the concentration profile can be sub-divided into two key phases, namely: (a) phase-1 stage whereby there is a consistent rise in its effluent concentration over a short period of time; and (b) phase-2 stage whereby the effluent's concentration gradient over time approaches a quasi-steady-state condition over long periods as building towards the filter's exhaustion stage.

During the initial state, the media grains (collector spheres) are in their relatively clean state, i.e. very minimum concentration of adsorbed contaminants at the spheres' boundaries (Ω_{fs}), and desorption flux of contaminants from the same boundaries is negligible. As net adsorption of contaminants occurs along the media depth during the initial state in (3.1.4), the average concentration at the spheres' boundaries will increase over time with respect to the following proposed relationship:

$$\frac{\partial c_s^*}{\partial t^*} = -\frac{1}{L} \frac{\partial S^*}{\partial x_i^*} \cdot \left(D_p^* \frac{\partial c^*}{\partial x_i^*} \right), \quad x^* \subset \Omega_{fs} \quad (3.1.8)$$

In (3.1.8), c_s^* increases over time which then leads to a transient reduction in the adsorber's removal efficacy as evident in the rise in its effluent concentration profile over a relatively short period of throughput units in phase-1 stage (Figure 1). In other words, the desorption flux inside the adsorber is becoming significant in (3.1.4) whereby k_{ads} and k_{des} are still within the same order of magnitude. Beyond a certain period, we hypothesize that c_s^* becomes close in magnitude as that of c^* leading to a near-equilibrium concentration state in phase-2 (Figure 1) as building towards the adsorber's exhaustion stage. A unique relationship between c^* and c_s^* will be proposed in the later section to analyze phase-2 stage.

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At the same time, k_{rem} and k_{det} in (3.1.4) are still within the same order of magnitude in phase-2 stage whereby there is a complex close balance between the adsorption (k_{rem}) and desorption (k_{det}) mechanisms taking place concurrently inside an adsorber. Prior to its exhaustion stage, net adsorption of contaminants is still taking place over phase-2 stage as the average normalized effluent concentration from the adsorber is still less than the value of unity, as shown in Figure 2.3.1. Note that the value of k_{rem} is greater than that of k_{det} but is still within the same order of magnitude during phase-2 stage. Intuitively, both k_{rem} and k_{det} are equivalent in value, i.e. equilibrium between the adsorption and desorption mechanisms, when the adsorber's exhaustion stage is attained whereby its average normalized effluent concentration equals to the value of unity for significant periods. These conditions provide the basis for the analytical modelling of the complex adsorption-desorption processes taking place inside adsorbers.

3.2. Normalization

To normalize the above defined representations associated with the respective clogging conditions, we adopt the following scaling variables: (i) $c^* = c_{eqm}c$; (ii) $t^* = Tt$; (iii) $u_i^* = Uu_i$; (iv) $x_i^* = lx_i$; (v) $p^* = Pp$; and (vi) $d^* = ld$; whereby T , U and P are the respective scales for the time, velocity and pressure parameters. c_{eqm} is assumed to scale to the order of magnitude inherent to the influent concentration (c_0) of contaminants being filtered through seepage filter, defined as:

$$c_{eqm} \sim O(c_0) \quad (3.2.1)$$

In (3.2.2), we define a dominant balance between the pressure gradient acting upon the depth filter and the viscous flow resistance around the collector spheres inside each periodic cell domain for all clogging conditions (physical, chemical, biological) being modelled.

$$\frac{P}{L} \sim O\left(\frac{vU}{l^2}\right) \quad (3.2.2)$$

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To derive the respective homogenized averaged representations for quantifying the respective clogging condition, different reaction time scales are proposed based on appropriate arguments. For physical clogging condition, the macroscale convection time scale of T_c , as defined in (3.2.3), is adopted as the clogging scenario is expected to take place over the filter's convection time scale as evident from previous experimental studies (Hajra et al., 2002; Zhou et al., 2012; Wang et al., 2012; Seifert et al., 2014; Page et al., 2014).

$$T_c = \frac{L}{U}, \quad (3.2.3)$$

On the contrary, the macroscale reaction (adsorption, desorption, etc.) time scales, defined in (3.2.4) and (3.2.5), are adopted to model the chemical and biological clogging conditions, respectively, inside depth filters.

$$T_{ads} = \frac{L}{k_{ads}}, \quad T_{des} = \frac{L}{k_{des}}, \quad O(T_{ads}) \cong O(T_{des}) \quad (3.2.4)$$

$$T_{att,fb} = \frac{L}{k_{m/p,fb}}, \quad T_{reaction,B} = \frac{L}{k_{m/p,reaction}}, \quad (3.2.5)$$

where T_{ads} and T_{des} are the respective time scale for adsorption and desorption of contaminants to take place at the spheres' boundaries, $T_{att,fb}$ the time scale for the contaminants/microbes to be attached at the boundary of the biofilm layer, i.e. interphase between the fluid and biofilm layer, and $T_{reaction,B}$ the time scale for the contaminants/microbes to undergo complex reaction processes within the thin reactive layer beneath the biofilm boundary.

In (3.2.4), both T_{ads} and T_{des} are taken to be within the same order of magnitude, as discussed earlier, for modelling the chemical clogging condition in adsorbers since previous studies (Rumynin et al., 2005; Mishra et al., 2013; Kyzas et al. 2014; Mishra., 2014; Rani and Sud., 2015) have justified that both processes are responsible for removing different types of contaminants via the net adsorption process (adsorption rate greater than desorption rate) in both batch and column tests. For convenience, T_{ads} will be used to normalize (3.1.1), (3.1.3) and (3.1.8) for modelling

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the chemical clogging condition in adsorbers. On the contrary, both $T_{att,fb}$ and $T_{reaction,B}$ are expected to be significantly different for modelling the biological clogging condition due to the differing length scales responsible for the respective processes (attachment at the interphase between fluid and porous biofilm layer and reaction within the same biofilm layer) inside the periodic cell domain. Intuitively, with respect to time, ε_a dictates the former process while the latter process is controlled by ε_b , which then results in $T_{att,fb} \cong \varepsilon_c T_{reaction,B}$.

The dimensionless microscale Peclet number (Pe_l), defined in (3.2.6), applies to all clogging scenarios, while the relationship between the macroscale Damköhler number, (D_L), in its general representation, and its microscale form is defined in (3.2.7).

$$Pe_l = \frac{Ul}{D_p^*} \quad (3.2.6)$$

$$D_L = \frac{kl}{\varepsilon D_p^*} = \frac{D_l}{\varepsilon}, \quad (3.2.7)$$

where D_L varies among the different clogging conditions being modelled, and k can represent any of the reaction rate coefficients ($k_{ads}, k_{des}, k_{abs}, k_{rem}$) for the specific type of clogging condition. Note that the diffusion coefficient in (3.2.7) remains an unknown a priori and its effective value in each clogging scenario can be calibrated via supervised learning with measured data in the later analysis.

Using the above assessments for normalization, we systematically derive the dimensionless representations for each clogging scenario and perform the multiscale perturbation analysis on them to derive their respective homogenized averaged representations from a defined volume averaging technique, as represented in (3.2.8), in the next 3 sub-sections.

$$\tilde{f} = \frac{1}{|\Omega|_V} \iiint_{|\Omega_f|(x,t)} f \, d\Omega \quad (3.2.8)$$

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where f represents a dimensionless quantity of concern inside the fluid phase of the periodic cell problem, $|\Omega|_V = l^3$ the fixed volume of the periodic cell, $|\Omega_f|(x, t)$ the changing volume of fluid inside the cell during the specific clogging stage, and $\tilde{f}$ the homogenized fluid property inside the cell derived from the volume averaging step of (3.2.8) over the cell's fluid phase.

The next three sub-sections present the respective homogenized averaged representations for quantifying the inherent fluid flow and mass transport problems responsible for the different clogging conditions. Readers are referred to the works of Chew and Law (2019a, 2019b) for the exact derivations of the respective representations to model the physical and chemical clogging conditions inside depth filters.

3.3. Homogenized representations to quantify physical clogging condition

To carry out the homogenization procedures, the following multiple-scale coordinates of x and $x' = \varepsilon x$ are first introduced, whereby x is the fast variable defined within the periodic cell and x' is the slow variable spanning across the macroscale depth filter. The perturbation expansions for the physical parameters (which are all cell-periodic) are expressed as follows

$$G = G^{(0)} + \varepsilon G^{(1)} + \varepsilon^2 G^{(2)} + \dots \quad (3.3.1)$$

where G can be p , c and u_i .

The following spatial derivative is also adhered to carry out the multiscale perturbation expansions of (3.1.1 – 3.1.4) and (3.1.6 – 3.1.7) subsequently.

$$\frac{\partial}{\partial x_i} \rightarrow \frac{\partial}{\partial x_i} + \varepsilon \frac{\partial}{\partial x'_i} \quad (3.3.2)$$

3.3.1. Fluid flow problem

Using (3.2.8), the homogenized effective equation in (3.3.3), derived at the ordering importance of ε from the combined normalized forms of (3.1.1 – 3.1.2), relates the

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spatial variation of the dimensionless seepage velocity (RHS of (3.3.3)) to the direct multiplication between the dimensionless outward velocity acting at the sphere's boundary (growth rate of the sphere) and the slowly changing cell's porosity (LHS of (3.3.3)), caused by the physical clogging of turbidity particles inside the depth filter over space and time.

$$\frac{|S(x, t)|}{|\Omega|_V} \left(\frac{\partial d}{\partial t} \right) = \frac{\partial u_i^{(0)}}{\partial x_{i'}} = - \frac{\partial}{\partial x_{i'}} \left(\tilde{k}_{ij}(x, t) \frac{\partial p^{(0)}}{\partial x_{j'}} \right) \quad (3.3.3)$$

where $\tilde{k}_{ij}(x, t)$ the slowly changing permeability of the cell problem over space and time.

3.3.2. Mass transport problem

Again, by using (3.3.1) and (3.3.2) to perform the multiscale perturbation expansion of the normalized form of (3.1.3) and then relating them to (3.1.6) and (3.1.7) in their normalized representations accordingly, we derive the homogenized averaged expressions of (3.3.4) and (3.3.5) (Chew and Law., 2019a), after using the volume averaging method from (3.2.8), which quantify the filter's physical clogging behavior at the ordering importance of ε and ε^2 respectively.

$$\theta(x, t) \frac{\partial c^{(0)}}{\partial t} + \tilde{u}_i^{(0)}(x, t) \frac{\partial c^{(0)}}{\partial x_{i'}} = -Pe_l^{-1} \frac{|S(x, t)|}{|\Omega|_V} \frac{1}{\beta} \frac{\partial d}{\partial t}, \quad (3.3.4)$$

$$\begin{aligned} \theta(x, t) \frac{\partial c^{(1)}}{\partial t} + \tilde{u}_i^{(0)}(x, t) \frac{\partial c^{(1)}}{\partial x_{i'}} + \tilde{u}_i^{(1)}(x, t) \frac{\partial c^{(0)}}{\partial x_{i'}} \\ = Pe_l^{-1} \theta(x, t) \frac{\partial}{\partial x_{i'}} \left(\frac{\partial c^{(0)}}{\partial x_{i'}} \right) - Pe_l^{-1} \frac{|S(x, t)|}{|\Omega|_V} D_{a,L} c^{(1)}, \end{aligned} \quad (3.3.5)$$

Note that $\theta(x, t)$ represents the filter's average global porosity which varies over space and time for generality. From (3.3.4 – 3.3.5), we can confirm that the homogenized fluid flow and mass transport problems are directly linked via the slowly changing seepage flow velocity parameter, i.e. $\tilde{u}_i^{(0)}(x, t)$, for modelling the filter's physical clogging condition. We then consider the following linear time-derivative of the averaged concentration parameter, i.e. $\tilde{c} = \theta(x, t)(c^{(0)} + \varepsilon c^{(1)} + \dots)$, as:

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$$\frac{\partial \tilde{c}}{\partial t} = \theta(x, t) \frac{\partial c^{(0)}}{\partial t} + \varepsilon \theta(x, t) \frac{\partial c^{(1)}}{\partial t} + O(\varepsilon^2) \quad (3.3.6)$$

By using (3.3.4) and (3.3.5), we derive (3.3.7) for (3.3.6), accurate up to $O(\varepsilon^2)$, which quantifies the averaged transport and trapping behavior of turbidity particles inside depth filters.

$$\frac{\partial \tilde{c}}{\partial t} = -\frac{\partial(\tilde{u}_i c)}{\partial x_{i'}} - D_{a,L} Pe_l^{-1} \frac{|S(x, t)|}{|\Omega|_V} c + \varepsilon Pe_l^{-1} \theta(x, t) \frac{\partial}{\partial x_{i'}} \left(\frac{\partial c}{\partial x_{i'}} \right) + O(\varepsilon^2), \quad (3.3.7)$$

During the effective filtration stage, trapping of turbidity particles is expected to be most significant near to the filter's injection point. Hence, spatial variation to the global filter's seepage velocity occurs, which then modifies (3.3.7) into:

$$\begin{aligned} \frac{\partial \tilde{c}}{\partial t} = & -\tilde{u}_i(x, t) \frac{\partial c}{\partial x_{i'}} - c \frac{|S(x, t)|}{|\Omega|_V} \frac{\partial d}{\partial t} - D_{a,L} Pe_l^{-1} \frac{|S(x, t)|}{|\Omega|_V} c + \varepsilon Pe_l^{-1} \theta(x, t) \frac{\partial}{\partial x_{i'}} \left(\frac{\partial c}{\partial x_{i'}} \right) \\ & + O(\varepsilon^2), \end{aligned} \quad (3.3.8)$$

To further simplify (3.3.8), we then assume quasi-steady-state physical clogging condition and one-dimensional filtration flow. (3.3.9), which is then extracted from the simplified form of (3.3.8), compares the respective terms at the leading order for modelling the physical clogging condition inside depth filters.

$$0 = -\tilde{u}_K(x_K, t) \frac{\partial c}{\partial x_{K'}} - c \frac{|S(x_K, t)|}{|\Omega|_V} \frac{\partial d}{\partial t} - D_{a,L} Pe_l^{-1} \frac{|S(x_K, t)|}{|\Omega|_V} c, \quad (3.3.9)$$

where x_K is along the downward seepage direction towards the filter's effluent discharge point. Using the homogenized Darcy's Law representation $(\tilde{u}_K(x_K, t) = -\tilde{k}(x_K, t) \frac{\partial p}{\partial x_{K'}})$ in its averaged form for unidirectional flow (Chew and Law., 2019a, 2019b), (3.3.9) is further modified into:

$$0 = \tilde{k}(x_K, t) \frac{\partial p}{\partial x_{K'}} \frac{\partial c}{\partial x_{K'}} - \frac{|S(x_K, t)|}{|\Omega|_V} \left(\frac{\partial d}{\partial t} + D_{a,L} Pe_l^{-1} \right) c, \quad (3.3.10)$$

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where $\tilde{k}$ is the average global permeability coefficient of the one-dimensional depth filter which varies slowly over space and time due to the physical clogging condition taking place.

Adhering to the influent's boundary condition of $c(0) = 1$, the exact solution to (3.3.10) can be expressed as:

$$\tilde{k}(x_K, t) = \frac{A(x_K, t)}{\ln(c) \left(\frac{\partial p}{\partial x_{K'}} \right)} x_{K'} + C_1 = - \frac{m(x_K, t)}{\left(\frac{\partial p}{\partial x_{K'}} \right)} x_{K'} + C_1, \quad (3.3.11)$$

whereby $m(x_K, t) = - \frac{A(x_K, t)}{\ln(c)}$ and $A(x_K, t) = \frac{|S(x_K, t)|}{|\Omega|_V} \left(\frac{\partial d}{\partial t} + D_{a,L} Pe_l^{-1} \right)$ which is linked to the filter's physical parameters responsible for its physical clogging condition. C_1 in (3.3.11) is an unknown integration constant which varies between 0 and 1 since $\tilde{k}(x_K, t)$ is a dimensionless parameter and too varies between 0 and 1. Note that $\ln(c)$ is always negative, i.e. $c < 1$, at the filter's effluent discharge point during its effective clogging stage, and $\frac{\partial p}{\partial x_{K'}}$ is also a negative quantity along the media depth as gravitational force controls the downward seepage flow direction.

In the later section, we model the filter's physical clogging condition with respect to its maximum dimensionless media depth, i.e. $x_K = \varepsilon^{-1}$, and demonstrate in quantitative details how supervised learning methods are adopted to train $m(\varepsilon^{-1}, t)$, from (3.3.11), with measured dataset extracted from the literature.

3.4. Homogenized representations to quantify chemical clogging condition

Likewise, (3.2.8) and (3.3.1 – 3.3.2) will be adopted to derive the homogenized averaged representations which model the fluid flow and mass transport problems responsible for the chemical clogging condition taking place in depth filters due to the net adsorption process, i.e. adsorption rate greater than desorption rate, of contaminants over time.

3.4.1. Fluid flow problem

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At the ordering importance of ε , (3.4.1) represents the homogenized dimensionless Darcy's Law derived from the combined normalized forms of (3.1.1 – 3.1.2) after the volume averaging step using (3.2.8) together with the multiscale perturbation analysis.

$$\tilde{u}_i^{(0)} = -\tilde{k}_{ij} \frac{\partial p^{(0)}}{\partial x_j'}, \quad (3.4.1)$$

where $\tilde{u}_i^{(0)}$ is the dimensionless average seepage velocity, and $\tilde{k}_{ij}$ the dimensionless average effective permeability tensor. Unlike from the physical clogging condition, $\tilde{k}_{ij}$ remains unchanged over time during the filter's chemical clogging stage as the analysis does not consider any transient variations to the spheres' initial diameters within the periodic cell domain.

At the next ordering importance of ε^2 , we obtain the following simplified form before volume averaging:

$$\frac{k_{fs} l}{v} \frac{\partial u_i^{(0)}}{\partial t} = -\frac{\partial p^{(1)}}{\partial x_i'} + \frac{\partial}{\partial x_j} \left(\frac{\partial u_i^{(1)}}{\partial x_j} \right) + \frac{\partial}{\partial x_j} \left(\frac{\partial u_i^{(0)}}{\partial x_j'} \right), \quad x \in \Omega_f \quad (3.4.2)$$

We shall later show, in quantitative details, that solving for the averaged value of $u_i^{(1)}$ in (3.4.2) is not important due to the inherent dynamics of the chemical clogging condition. In addition, analysing the flow problem at the higher orderings of ε^3 and beyond is insignificant due to the smallness of ε . For large-scale porous media systems, the ordering of ε^3 is close to 10^{-12} which is insignificant for engineering predictions. In general, the derived homogenized averaged solutions for quantifying the macroscale flow and transport problems in depth filters (porous media systems) are expected to approach the error accuracy of $O(\varepsilon^3)$ in all clogging scenarios.

3.4.2. Mass transport problem

At the leading order, it can easily be shown that $c^{(0)}$ is independent of the microscale spatial variations (Chew and Law., 2019b) from the multiscale perturbation expansions

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of the combined normalized forms of (3.1.3 – 3.1.4). Hence, $c^{(0)}$ is taken as a constant value which remains invariant over time.

At the next ordering importance of ε , we obtain the following homogenized expression from the combined normalized forms of (3.1.3 – 3.1.4) with the volume averaging step of (3.2.8) (Chew and Law., 2019b).

$$Pe_l \tilde{u}_i^{(0)} \frac{\partial c^{(0)}}{\partial x_{i'}} = - \frac{|S|}{|\Omega|_V} (D_{ads,L} c^{(0)} - D_{des,L} c_s^{(0)}), \quad (3.4.3)$$

At the same ordering importance, we again adopt (3.2.8) to derive the homogenized expression of (3.4.4) for (3.1.8) which quantitatively shows that the transient rise of the surface concentration of contaminants at the spheres boundaries, with respect to the leading order (ε^0), is directly linked to the concentration gradient in the fluid phase around the sphere boundary at the current order of ε during the adsorber's chemical clogging stage.

$$D_{ads,L} \frac{\partial c_s^{(0)}}{\partial t} = - \frac{\frac{\partial S}{\partial x_i}}{|\nabla S|} \cdot \left(\frac{\partial c^{(1)}}{\partial x_i} \right), \quad (3.4.4)$$

Proceeding to the next order of ε^2 , we derive the following homogenized expressions from the volume averaging method (Chew and Law., 2019b) for the combined normalized representations of (3.1.3) and (3.1.4), and (3.1.4) and (3.1.8) respectively.

$$\begin{aligned} \theta D_{ads,L} \frac{\partial c^{(0)}}{\partial t} + Pe_l \left(\tilde{u}_i^{(0)} \frac{\partial c^{(1)}}{\partial x_{i'}} + \tilde{u}_i^{(1)} \frac{\partial c^{(0)}}{\partial x_{i'}} \right) \\ = \theta \frac{\partial}{\partial x_{i'}} \left(\frac{\partial c^{(0)}}{\partial x_{i'}} \right) - \frac{|S|}{|\Omega|_V} (D_{ads,L} c^{(1)} - D_{des,L} c_s^{(1)}), \end{aligned} \quad (3.4.5)$$

$$D_{ads,L} \frac{\partial c_s^{(1)}}{\partial t} = D_{ads,L} c^{(1)} - D_{des,L} c_s^{(1)}, \quad (3.4.6)$$

$\frac{\partial c^{(0)}}{\partial x_{i'}}$ in (3.4.5) can be neglected since $c^{(0)}$ has previously been shown to be a constant value along the media depth. Hence solving for $\tilde{u}_i^{(1)}$ in (3.4.5) becomes unnecessary.

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We again assume the linear time-derivative of the averaged fluid concentration, i.e. $\tilde{c} = \theta(c^{(0)} + \varepsilon c^{(1)} + \dots)$, from (3.3.6) without considering any spatial and transient variations to the periodic cell's porosity due to the chemical clogging condition.

By substituting (3.4.3) and (3.4.5) into (3.3.6), the following approximated expression can be derived which models the combined transient advection-diffusion-reaction mechanisms inside macroscale adsorbers.

$$\varepsilon^2 \frac{\partial \tilde{c}}{\partial t} \approx -\varepsilon \frac{Pe_l}{D_{ads,L}} \frac{\partial(c\tilde{u}_i)}{\partial x_i'} + \varepsilon^2 \frac{\theta}{D_{ads,L}} \frac{\partial}{\partial x_i'} \left(\frac{\partial c}{\partial x_i'} \right) - \varepsilon \frac{|S|}{|\Omega|_V} \left(c - \frac{D_{des,L}}{D_{ads,L}} c_s \right), \quad (3.4.7)$$

At the same time, the averaged homogenized representation for the normalized form of (3.1.8) is expressed as:

$$\frac{\partial c_s}{\partial t} + \frac{D_{des,L}}{D_{ads,L}} c_s = c, \quad (3.4.8)$$

(3.4.8) represents a first-order inhomogeneous equation subject to the initial condition of $c_s(t = 0) = 0$ under the initial clean state of the media grains. We avoid solving for the complex effective diffusion coefficient within the periodic cell problem for (3.4.3) and (3.4.5) due to the following reasons: (a) present unknowns in $D_{ads,L}$, $D_{des,L}$ and Pe_l (field conditions) which capture the coexisting adsorption and desorption processes taking place inside a macroscale adsorber; and (b) quantifying the periodic cell's random configuration of spheres, as shown previously in Figure 2.3.1, on the effective diffusion coefficient is difficult. In the following, we provide the key homogenized averaged representations which model the respective behaviours of both phase-1 and phase-2 stages, as described earlier, in operating adsorbers.

Phase-1 stage: $\frac{\partial \tilde{c}}{\partial t} \neq 0$

We first compare the terms of (3.4.7) at the ordering importance of ε^2 in (3.4.9) which describes the transient variation of the fluid concentration due to the diffusion mechanism solely during an adsorber's chemical clogging stage.

$$\frac{\partial \tilde{c}}{\partial t} = \frac{\theta}{D_{ads,L}} \frac{\partial}{\partial x_i'} \left(\frac{\partial c}{\partial x_i'} \right), \quad (3.4.9)$$

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whereby (3.4.9) is subjected to the following initial and boundary conditions:

$$c(t = 0) = f(x_i'), \quad 0 \leq x_i' \leq \varepsilon^{-1} \quad (3.4.10a)$$

$$c(x_i' = 0) = 1, \quad t \geq 0 \quad (3.4.10b)$$

$$c(x_i' = \varepsilon^{-1}) = \phi(t), \quad t \geq 0 \quad (3.4.10c)$$

where $f(x_i')$ is an unknown function of the adsorber's media depth, and $\phi(t)$ represents the unknown effluent discharge concentration profile at the maximum media depth which varies over time during operations. No priori imposition of the end-boundary in (3.4.10c) is introduced in this study.

Phase-2 stage: $\frac{\partial \tilde{c}}{\partial t} \rightarrow 0; c \geq c_s$

In phase-2 stage, both adsorption and desorption processes are occurring concurrently inside the macroscale adsorber as building towards its exhaustion stage, of which both k_{ads} and k_{des} in (3.4.7) are still within the same order of magnitude as discussed earlier. Overall, a net adsorption of contaminants ($k_{ads} > k_{des}$) is still taking place as long as c remains less than unity (see Figure 2.3.1). The extracted terms of (3.4.7) at the ordering of ε^1 , as shown in (3.4.11), quantifies the spatial variation of the contaminants' concentration within the fluid phase along the adsorber's media depth, due to the concurrent adsorption and desorption of the contaminants taking place at the spheres' boundaries.

$$\frac{Pe_l}{D_{ads,L}} \frac{\partial(c\tilde{u}_i)}{\partial x_i'} = -\frac{|S|}{|\Omega|_V} \left(c - \frac{D_{des,L}}{D_{ads,L}} c_s \right), \quad (3.4.11)$$

In phase-2 stage, the near-equilibrium concentration state occurs whereby the surface concentration and fluid concentration can be related via the following proposed mass balance relationship:

$$\gamma \cong \frac{c(\theta l^3)}{(\theta l^3)c + c_s(1 - \theta)l^3}, \quad (3.4.12)$$

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where γ is the assumed porosity of a monolayer packing of contaminants in the fluid phase around the grain/sphere surface. Note that θ and l respectively represent the known global porosity of the adsorber and the characteristic length of the defined periodic cell problem.

The slow transient variations of c in the fluid phase during phase-2 stage can be ascribed to the reversible adsorption process (near-equilibrium concentration state) which thus qualifies the maximum possible monolayer density to around 90% coverage of the collector sphere's surface area (Feder, 1980; Johnson, 1995; Pennell, 2016). Hence, the value of γ can be computed based on the surface area considerations around the collector spheres within each periodic cell domain as follows:

$$\gamma \cong \frac{A_{monolayer}}{A_{monolayer} + A_{spheres}}, \quad (3.4.13)$$

where A_{sphere} and $A_{monolayer}$ are the surface area of the ideal collector spheres and the monolayer packing around the spheres' boundaries respectively within each cell domain. $A_{monolayer}$ is assumed as $0.9(A_{sphere})$ as discussed above. Thus, γ is estimated to be 0.474 from (3.4.13). Substituting the combined form of (3.4.12 – 3.4.13) into (3.4.11) results into:

$$\frac{\varepsilon U}{k_{ads}} \left(c \frac{\partial \tilde{u}_K}{\partial x_K'} - \tilde{k} \frac{\partial p}{\partial x_K'} \frac{\partial c}{\partial x_K'} \right) = - \frac{|S|}{|\Omega|_V} \left(1 - \frac{k_{des}}{k_{ads}} \frac{(1-\gamma)\theta}{\gamma(1-\theta)} \right) c, \quad (3.4.14)$$

whereby $\tilde{k}$ is the average global permeability coefficient of an adsorber which does not vary over space and time during its chemical clogging stage.

No spatial variation of the seepage velocity ($\tilde{u}_K$) is considered inside adsorbers during their chemical clogging stage, which then modifies (3.4.14) into:

$$\frac{\partial c}{\partial x_K'} = -\beta c, \quad (3.4.15)$$

where $\beta = - \frac{k_{ads} \frac{|S|}{|\Omega|_V} \left(1 - \frac{k_{des}}{k_{ads}} \frac{(1-\gamma)\theta}{\gamma(1-\theta)} \right)}{\frac{l}{L} U \left(\tilde{k} \frac{\partial p}{\partial x_K'} \right)}.$

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Note that both $\frac{\partial c}{\partial x_K'}$ and $K \frac{\partial p}{\partial x_K'}$ are again negative quantities in the compacted term of β for downward seepage filtration flow in adsorbers. By using the known inlet boundary condition of (3.4.10b), the exact solution to (3.4.15) can be expressed as:

$$c = e^{-\beta x_K'}, \quad (3.4.16)$$

Likewise, in the later section, we demonstrate in quantitative details of how various supervised learning methods can be adopted to calibrate β with respect to different varied operating conditions for adsorbers at their maximum media depth of $x_K = \varepsilon^{-1}$.

Chapter 4: Pre-processing step to couple theoretical modelling with supervised machine learning techniques

Chapter Overview:

This chapter describes, in quantitative details, the prior pre-processing steps undertaken to couple the built theoretical models, i.e. homogenized averaged representations derived from Sections 3.3 and 3.4 with various supervised machine learning techniques which include regression analysis, neural network modelling, etc., for modelling each specific clogging condition in depth filters. In addition, data extractions from relevant literature, followed by appropriate augmentation steps, are carried out to build up the pool of training instances for calibrating the respective predictive model tailored to each clogging scenario.

Sections 4.1 and 4.2 describe in quantitative details the pre-processing procedures undertaken to couple the built theoretical models with supervised machine learning techniques, followed by their respective data processing and augmentation steps to model the physical and chemical clogging condition respectively.

4.1. Pre-processing procedures for modelling physical clogging condition

Using dimensional analysis, we model $\tilde{k}(x_K, t)$ in (3.3.11) as a function of the following known physical parameters: (i) initial grain size (d_0^*); (ii) media depth (L_m); (iii) hydraulic loading rate (V_s); (iv) influent's concentration (c_0); (v) size of turbidity particles (d_p); (vi) density of turbidity particles (ρ_p); (vii) gravitational acceleration (g); (viii) kinematic viscosity (ν); and (ix) filtration time (t^*). Adopting the repeating variables of ρ_p , g and L_m for the Buckingham pi-group theorem, the following pi-terms are obtained as:

$$\begin{aligned} \pi_1 = \tilde{k}(x_K, t), \quad \pi_2 = \frac{d_0^*}{L_m}, \quad \pi_3 = \frac{V_s}{(L_m)^{0.5} g^{0.5}}, \quad \pi_4 = \frac{c_0}{\rho_p}, \quad \pi_5 = \frac{t^* g^{0.5}}{(L_m)^{0.5}}, \\ \pi_6 = \frac{d_p}{L_m}, \quad \pi_7 = \frac{\nu}{(L_m)^{1.5} g^{0.5}} \end{aligned} \quad (4.1.1)$$

For convenience, the physical clogging problem is linearized by taking the natural logarithm on both sides of (3.3.11) to obtain:

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$$\ln(\tilde{k}(x_K, t)) = \ln\left(-\frac{m(x_K, t)}{\frac{\partial p}{\partial x_K'}} x_K' + C_1\right) = B(x_K, t), \quad (4.1.2)$$

The lumped term of $B(x_K, t)$ is again modelled with the same physical parameters of (i – ix), hence adhering to the same derived pi-terms from (4.1.1). Appropriate re-arrangement of the variables within the pi-terms from (4.1.1) is also carried out to build the respective quantitative relationship between each independent pi-term and $B(x_K, t)$ whereby each condition generally leads to higher $\ln(\tilde{k})$ values over time, i.e. gradual reduction of $\tilde{k}$, in (4.1.2).

- i. Invert $\frac{d_0^*}{L_m}$ as smaller grains tend to result in higher trapping efficacy of the turbidity particles inside the seepage filter
- ii. Higher V_s values increase the mass flux of turbidity particles into the filter which result in greater mass of particles to be trapped per unit time
- iii. Higher c_0 values have the tendency for higher mass/volume of turbidity particles to be trapped inside the filter
- iv. Smaller ρ_p values usually result in greater number of turbidity particles to be trapped inside the filter for each mass/volume of influent filtered
- v. Invert $\frac{d_p}{L_m}$ as smaller-sized turbidity particles tend to result in greater number of particles to be trapped inside the filter for each mass/volume of influent filtered
- vi. Invert $\frac{\nu}{(L_m)^{1.5} g^{0.5}}$ as lower fluid viscosity tends to result in higher removal efficacy of turbidity particles inside the filter for each mass/volume of influent filtered

By adhering to the above-mentioned conditions, $B(x_K, t)$ can be quantified as follows:

$$B(x_K, t) = f\left(\frac{L_m}{d_0^*}, \frac{V_s}{(L_m)^{0.5} g^{0.5}}, \frac{t^* g^{0.5}}{(L_m)^{0.5}}, \frac{c_0}{\rho_p}, \frac{L_m}{d_p}, \frac{(L_m)^{1.5} g^{0.5}}{\nu}\right) \quad (4.1.3)$$

In (4.1.3), the pre-processed input layer is thus built for supervised learning algorithms in the following ways: (a) six independent input features whereby each

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unique dimensionless pi-term represents an input feature; or (b) adopt the simplest monomial form for (4.1.3) in (4.1.4) whereby it represents a compacted input feature.

$$B(x_K, t) = n_1 \left(\frac{L_m}{d_0^*} \cdot \frac{V_s}{(L_m)^{0.5} g^{0.5}} \cdot \frac{t^* g^{0.5}}{(L_m)^{0.5}} \cdot \frac{c_0}{\rho_p} \cdot \frac{L_m}{d_p} \cdot \frac{(L_m)^{1.5} g^{0.5}}{v} \right)^{n_2} \quad (4.1.4)$$

whereby n_1 and n_2 are unknown calibration constants with specific emphasis of n_1 being the weighted average of the compacted representation as the only input feature. Note that (4.1.4) can have a biased constant term during the model calibration step.

To model the depth filter's physical clogging condition in the later stage, we extract raw measured data from the literature which examine the physical clogging condition in column tests, namely from the experimental studies of Zhou et al. (2009) and Wang et al. (2012) as illustrated in non-linearized (Figure 4.1.1) and linearized (Figure 4.1.2) forms respectively.

Figure 4.1.1. Non-linearized representation of raw dataset extracted from Zhou et al. (2009) and Wang et al. (2012); the respective figures in the actual papers for the extracted raw dataset are indicated accordingly.

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Figure 4.1.2. Linearized (by taking natural logarithm) representation of raw dataset extracted from Zhou et al. (2009) and Wang et al. (2012); the respective figures in the actual papers for the extracted raw dataset are indicated accordingly.

Prior to training, the number of raw measured instances is limited as evident in both Figures 4.1.1 and 4.1.2 which thus hinders the initial training step. To enlarge the size of the present training dataset, we adhere to the following data augmentation procedures for the linearized raw dataset from Figure 4.1.2.

- i. Extract the available data points for $\ln(\tilde{k}(\varepsilon^{-1}, t))$ at the maximum media depth associated from a defined training period in each experiment.
- ii. Perform linear regression analysis of $\ln(\tilde{k}(\varepsilon^{-1}, t))$ over time of the defined training period from step (i).
- iii. Check the respective high coefficient of determination (R^2) values; ensure that R^2 should be of minimum value of 0.90 (a defined arbitrary value in our analysis). If so, proceed to step (v).
- iv. Attempt a higher-order regression analysis or other types of machine learning models of the extracted measured data from step (i) and perform step (ii – iii) again. Note that very high ordering degrees are avoided whenever possible to prevent overfitting of the augmented dataset during model training.
- v. Adopt the derived fitting model from step (ii) to interpolate more training data points for $\ln(\tilde{k}(\varepsilon^{-1}, t))$ associated with the same training period defined from step (i) by using a finer time-step (resolution).

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- vi. For the defined time-step from step (iv), augment the quantity of data points, to the computed quantity of [(total training period)/(time-step)] associated with the total defined training period in throughput units defined from step (i).

The above steps (i – vi) are thus adopted to generate a suitable amount of training instances for each of the referenced experiments of Zhou et al. (2009) and Wang et al. (2012). In the later section, the augmented training instances are adopted to perform supervised learning, via the use of a shallow deep multi-layered neural network (NN) architecture, of the proposed model in (4.1.4) to quantify the depth filter's physical clogging condition in the respective referenced experiments.

4.2. Pre-processing procedures for modelling chemical clogging condition

Likewise, using dimensional analysis, β in (3.4.16) is modelled as a function of an adsorber's known physical parameters as follows: (i) initial grain size (d_0^*); (ii) media depth (L_m); (iii) hydraulic loading rate (V_s); (iv) influent's concentration (c_0); (v) size of contaminants (d_p); (vi) bulk density of contaminants (ρ_p); (vii) BET surface area per unit mass of media grains (A_g); (viii) kinematic viscosity (ν); and (ix) period of phase-2 (see Figure 3.1.2) as measured in days (t^*). By adopting the repeating variables of ρ_p , V_s and d_0^* for the Buckingham pi-group theorem, the following pi-terms are obtained as:

$$\begin{aligned} \pi_1 &= \frac{k_{ads}}{V_s}, & \pi_2 &= \frac{d_p}{d_0^*}, & \pi_3 &= \rho_p A_g d_0^*, & \pi_4 &= \frac{c_0}{\rho_p}, & \pi_5 &= \frac{t^* V_s}{d_0^*}, & \pi_6 &= \frac{L_m}{d_0^*}, \\ \pi_7 &= \frac{\nu}{d_0^* V_s} \end{aligned} \quad (4.2.1)$$

Again, appropriate re-arrangement of the different variables is carried out within the respective pi-terms in (4.2.1) to build the respective quantitative relationship between each independent pi-term and k_{ads} , whereby each unique condition leads to higher k_{ads} value, i.e. higher adsorption rate of contaminants at the grains' surfaces.

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- i. Smaller d_0^* values provide greater surface area per unit volume of media grains for adsorption to occur
- ii. Larger L_m values provide greater amount/volume of media grains inside the filter for adsorption to occur
- iii. Larger A_g values provide greater surface area per unit mass of media grains for adsorption to occur
- iv. Higher c_0 values result in higher mass flux of contaminants entering the adsorber, hence increasing the probability of adsorption of contaminants to materialize
- v. Smaller ρ_p values result in greater number of contaminants to be adsorbed inside the filter for each unit mass/volume of influent filtered effectively
- vi. Higher V_s values result in higher mass flux of contaminants entering the adsorber, hence increasing the probability of adsorption of contaminants to materialize
- vii. Larger d_p values should increase the probability of contact, i.e. adsorption, of the contaminants with the surfaces of the media grains
- viii. Lower ν values should increase the probability of contact, i.e. adsorption, of the contaminants with the surfaces of the media grains

In summary, $\frac{k_{ads}}{V_s}$ can be modelled as follows:

$$\frac{k_{ads}}{V_s} = f\left(\frac{d_p}{d_0^*}, \rho_p A_g d_0^*, \frac{c_0}{\rho_p}, \frac{t^* V_s}{d_0^*}, \frac{L_m}{d_0^*}, \frac{d_0^* V_s}{\nu}\right) \quad (4.2.2)$$

Again, for simplicity, we consider the simplest monomial relationship for (4.2.2) in the following form:

$$\frac{k_{ads}}{V_s} = n_1 \left(\frac{d_p}{d_0^*} \cdot \rho_p A_g d_0^* \cdot \frac{c_0}{\rho_p} \cdot \frac{t^* V_s}{d_0^*} \cdot \frac{L_m}{d_0^*} \cdot \frac{d_0^* V_s}{\nu} \right)^{n_2} \quad (4.2.3)$$

whereby n_1 and n_2 are unknown calibration coefficients with specific emphasis of n_1 being the weighted average of the compacted representation.

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Raw measured data, which examined the adsorption behavior in column tests (Treumann et al., 2014; Zhao et al., 2016), is extracted accordingly to provide the necessary training instances for calibrating (4.2.3) via supervised learning methods in the later stages. The extracted dataset is plotted in Figures 4.2.1 and 4.2.2 respectively for illustrations. Likewise, data-deficiency is again present in phase-2 stage of Figures 4.2.1 and 4.2.2 as shown. Hence, the following data augmentation procedures are undertaken to enlarge the pool of training instances to calibrate (4.2.3) in the later stage.

- i. From the identified phase-2 region in each experiment with respect to Figures 4.2.1 and 4.2.2 accordingly, the available data points for c are extracted at the maximum media depth associated from the pre-defined training period of phase-2 stage in throughput units.
- ii. Perform linear (first-order characteristic) regression analysis of c over time of the defined training period from step (i).
- iii. Check the respective coefficient of determination (R^2) values from step (i); ensure that the minimum R^2 value is least 0.90 (a defined arbitrary value in our analysis) or greater. If so, proceed to step (iii), else repeat step (i) with the next ordering degree till R^2 value is least 0.90 or greater. Note that very high ordering degrees are avoided whenever possible to prevent overfitting.
- iv. Adopt the derived fitting (linear or higher ordering degree) model from step (ii) to interpolate more training data points for c by using a finer time-step (resolution) associated with the total phase-2 period in throughput units as defined from step (i).
- v. For the defined time-step from step (iv), augment the quantity of data points, to the computed quantity of $[(\text{total phase-2 period})/(\text{time-step})]$ associated with the total phase-2 period in throughput units defined from step (i).

The respective throughput units for phase-2 stage in the referenced experiments (Treumann et al., 2014; Zhao et al., 2016) range between 0.5 to 1.6 and 0.15 ~ 0.20 to 0.9 in Figures 4.2.1 and 4.2.2 respectively. The above-mentioned data augmentation procedures (i – v) are thus adhered to generate a suitable amount of training instances for each of the referenced experiments. The augmented pool of

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training data is then adopted in the later section to train the proposed model of (4.2.3) for quantifying the concurrent adsorption-desorption processes taking place inside adsorbers which contributes to their chemical clogging condition over time.

Figure 4.2.1. Extracted data from Treunmann et al. (2014) studies for measured concentration profile for the adsorption of colloids in column tests.

Figure 4.2.2. Extracted data from Zhao et al. (2016) studies for measured concentration profile for the adsorption of ammonium ion in column tests.

Chapter 5: Numerical model development for supervised learning of clogging condition in rapid depth filters

Chapter Overview:

The contents of this chapter are extracted from three papers (Chew and Law., 2017, 2018a, 2019c) in the Applied Energy Journal and Energy Procedia. The proposed analytical method of coupling the homogenization theory with multiscale perturbation analysis, as described in Chapter 3, only models the mass transport of contaminants in depth filters under creeping flow conditions. To model the rapid flow condition inside depth filters, whereby the microscale Reynolds number is greater than the value of unity, numerical methods are instead adopted for analysing the filters' clogging behavior over time. This thesis report considers physical clogging to be most significant in rapid depth filters due its low residence fluid time. Hence, chemical and biological clogging conditions, which are more likely to be caused by creeping flow conditions, are expected to be insignificant in rapid filters.

In summary, this chapter describes, in quantitative details, the systematic development of two unique numerical tools, namely: (a) Dynamical Rapid Filtration Model (DRFM); and (b) Recurrent Neural Network coupled with Long-Short-Term-Memory cells (RNN-LSTM), to model the complex physical clogging condition taking place inside rapid depth filters. The primary objective of the proposed models is to estimate the rapid filters' direct energy gradient incurred over time, by incurring sufficiently low error risk between the model's predictions and respective measured values in economic terms, during the filters' effective physical clogging stages. By doing so, predictive maintenance can be performed for operating rapid filters which can provide long-term energy savings and greenhouse gases (GHG) reduction on the industry scale.

Chapters 5.1 and 5.2 respectively describe the pre-processing steps undertaken to develop DRFM and RNN-LSTM to quantify rapid filters' direct energy gradient incurred during their effective clogging stages for optimal predictive maintenance acts.

5.1. Development of Dynamical Rapid Filtration Model (DRFM)

DRFM models rapid depth filters' effective clogging stages by assuming transient growth of the media's effective grain size inside the filters, with respect to the traditional

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volume conservation principle (Chew and Law., 2018). As trapping of turbidity particles is expected to be most significant near the filter's entrance, the growth rate of the media grains is taken to be decreasing along the depth of the media, i.e. bigger grains in the upper regions of the rapid filter. DRFM assumes a modified Yao's model (Yao and O' Melia, 1968; Yao et al., 1971) by modelling the growing effects of the media size on the filter's direct energy gradient performance due to the transient effective removal of turbidity particles via the interception and gravitational sedimentation mechanisms. Both straining and inertial impaction mechanisms are assumed to be lumped with interception. Readers are referred to Appendix A for the exact mathematical derivations in DRFM for predicting the filter's direct energy gradient incurred over time (dimensionless quantity) due to effective clogging, defined as:

$$(\Delta H)_t = \frac{H_t - H_0}{H_0}, \quad (5.1.1)$$

where H_t is the filter's energy loss incurred at time (t), and H_0 the filter's initial energy loss at $t = 0$ incurred at the filter's maximum media depth.

The turbidity particles removed inside rapid filters are typically within the size range of 20 to 100 μ m or larger (Tehowater, 2017). Therefore, both diffusion and electrostatic attraction mechanisms are neglected for rapid filtration considerations. In DRFM, a unique length scale between the respective sizes of a singular media grain and a trapped turbidity particle is proposed to account for the particle size effect on the filter's direct energy gradient performance over time (Chew and Law., 2018). To the best of our knowledge, this empirical ratio has not been introduced before.

The input features into DRFM can be classified into controlled and non-controlled operational physical parameters which directly affect the filter's direct energy gradient performance during effective clogging. The former component consists of: (a) filter's hydraulic loading rate (V_s); (b) fluid's dynamic viscosity (μ_{in}); (c) average diameter of turbidity particle (d_p); (d) filter's media depth (L_m); and (e) filter's initial grain size (d_0^*), while the latter component comprises of: (a) average influent's concentration of turbidity particles (c_0); and (b) bulk density of influent's concentration of turbidity particles (ρ_p). Additional assumptions are also made for DRFM's applicability, namely:

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(a) d_p is quantified by the dominant particle size within the influent source; and (b) exceedance in the rapid filter's direct energy gradient occurs before exceedance in the effluent concentration for breakthrough criteria to initiate the maintenance act. Readers are referred to Chew and Law (2018) for further quantitative and qualitative details of DRFM for modelling rapid filters' direct energy gradient incurred due to effective physical clogging of turbidity particles over time.

5.2. Development of RNN-LSTM

In contrast to DRFM, recurrent neural network (RNN) coupled with long-short-term-memory (LSTM) cells are adopted to build RNN-LSTM. RNN-LSTM is based upon the shallow deep-learning concept which will be demonstrated later. Again, the same controlled and non-controlled physical parameters as listed in the previous sub-section for developing DRFM, together with filtration time (t^*) and gravitational acceleration (g) of $9.81m/s^2$ in value, are adhered to build RNN-LSTM. Note that H_0 is not considered as an input feature as the focus of RNN-LSTM (together with DRFM) is to account for the additional energy loss incurred by rapid filters during their effective filtration stages. ρ_p , g and L_m are selected as the repeating variables for the dimensional analysis, via the Buckingham pi-group theorem, due to the following reasons: (a) range of extracted values for ρ_p and L_m from the literature are within the same order of magnitude and can be measured easily on-field; and (b) g is a known constant. By doing so, the following dimensionless pi-terms are derived as follows:

$$\pi_1 = f(\pi_2, \pi_3, \pi_4, \pi_5, \pi_6, \pi_7), \quad (5.2.1)$$

$$\begin{aligned} \pi_1 &= (\Delta H)_t, & \pi_2 &= \frac{V_s}{(L_m)^{1/2} g^{1/2}}, & \pi_3 &= \frac{d_p}{L_m}, & \pi_4 &= \frac{t g^{1/2}}{(L_m)^{1/2}}, & \pi_5 &= \frac{d_0^*}{L_m}, \\ \pi_6 &= \frac{c_0}{\rho_p}, & \pi_7 &= \frac{\mu_{in}}{\rho_p (L_m)^{3/2} g^{1/2}} \end{aligned} \quad (5.2.2)$$

To reduce the feature space for RNN-LSTM, appropriate physical arguments are made to build the model's pre-processed input layer for modelling rapid filters' direct energy gradient metric over time $((\Delta H)_t)$ as measured in (5.1.1). Generally, higher

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trapping efficacy of turbidity particles inside the rapid filter per unit time leads to higher $(\Delta H)_t$ values.

- Invert $\frac{d_0^*}{L_m}$ which resulting term represents a common design criterion for depth filters and typically ranges between 1000 and 2000 in value (Crittenden et al., 2012; Voutchkov, 2012). The inversion also makes intuitive sense as smaller grain sizes result in smaller global porosity inside the depth filter, hence leading to higher trapping efficacy of each unit mass/volume of turbidity particles over time.
- ρ_p is expected to be inversely correlated to $(\Delta H)_t$ as smaller ρ_p value generally results in greater number of turbidity particles being trapped inside the filter per unit mass/volume of influents filtered effectively.
- V_s is expected to be directly correlated to $(\Delta H)_t$ as higher V_s values lead to higher mass influx of turbidity particles entering the depth filter, hence increasing the quantities of particles being effectively trapped inside the filter over time for every unit mass/volume of influents filtered.
- Invert $\frac{\mu_{in}}{\rho_p(L_m)^{3/2}g^{1/2}}$ as lower viscosities (due to higher fluid temperatures) improve the probability of contact of the turbidity particles with the media grains which further enhances the trapping efficacy of particles inside the filter over time for every unit mass/volume of influents filtered.
- Invert $\frac{d_p}{L_m}$ as $(\Delta H)_t$ is inversely proportional to the particle size (O'Melia and Ali., 1979; Mackie and Bai., 1992; Darby et al., 1992; Veerapaneni and Wiesner., 1993; Boller and Kavanaugh., 1995; Veerapaneni and Wiesner., 1997; Wiesner, 1999; Chew and Law., 2018) with respect to the total surface area of each unit mass/volume of turbidity particles being trapped effectively inside the depth filter over time.

Two possible types of the pre-processed input layer are considered for building RNN-LSTM, namely: (a) a total of 6 input features whereby each feature represents each dimensionless pi-term from (5.2.2); and (b) a singular input feature in (5.2.3) which represents a compact monomial relationship of all pi-terms from (5.2.2). Both (a) and (b) result in a many-to-many LSTM model which tracks the transient development of an arbitrary depth filter's direct energy gradient incurred at every defined time-interval, i.e. time-step, during the filter's effective filtration period.

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$$(\Delta H)_t = C_1 \left(\frac{V_s}{(L_m)^{1/2} g^{1/2}} \cdot \frac{L_m}{d_p} \cdot \frac{t g^{1/2}}{(L_m)^{1/2}} \cdot \frac{L_m}{d_0^*} \cdot \frac{c_0}{\rho_p} \cdot \frac{\rho_p (L_m)^{3/2} g^{1/2}}{\mu_{in}} \right)^{C_2}, \quad (5.2.3)$$

where C_1 and C_2 are unknown calibration constants.

Feeding a compacted input feature of (5.2.3) into RNN-LSTM unrolls the hybrid varied effects of the defined physical parameters, through sufficiently small time-steps, for modelling rapid filters' direct energy gradient over time. Continuous calibration of the specific weightage inherent to (5.2.3) is also performed at every time-step which cannot be performed by DRFM from our previous sub-section. Shallow deep RNN-LSTM model is built upon three stacked layers of LSTM cells coupled with dropout regularization which value ranges between 0 and 1. Figure 5.2.1 illustrates the many-to-many RNN-LSTM model structure adopted whereby there are 3 LSTM layers at each time-step and each layer contains 50 neural nodes. A dropout value of 0.2 is adhered for all LSTM cells.

Figure 5.2.1. Illustration of many-to-many RNN-LSTM model.

At every time-step during each epoch run, the final dense layer contains only a single node for computing the output value as RNN-LSTM is only concerned with modelling the transient variations of $(\Delta H)_t$ due to effective physical clogging conditions. RNN-LSTM avoids an overkill scenario of using deep learning methods as

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it leverages on a singular compacted input feature into the stacked hidden layers of neurons in the LSTM cells to track the transient development of $(\Delta H)_t$ over sufficiently small step sizes. In addition, using a compacted input feature of (5.2.3) compacts the error uncertainties, attributing from the different physical parameters, into in-built calibration coefficients of C_1 and C_2 derived from the earlier dimensional analysis step.

Adam optimizer is used to compile the RNN-LSTM model which has been shown to result in high model's accuracy during the training step, as compared to other available optimizers (Brownlee, 2017). A grid search algorithm is also adhered to determine the optimal set of hyper-parameters for training RNN-LSTM, namely: (a) batch size; (b) number of epochs; and (c) learning rate, to minimize the implemented cost function (mean-squared-error metric) with respect to the calibrated coefficients in (5.2.3) at each epoch. The following range of values are attempted for each of the above-mentioned hyper-parameter for training RNN-LSTM.

- i. Number of batch size – 1, 2, 4, 8, 16, 32
- ii. Number of epochs – 50, 100, 150
- iii. Learning rate – 0.001, 0.01, 0.1

For evaluating RNN-LSTM, DRFM, and the proposed analytical models (from the combined Chapters 3 and 4), the following cost-functions of *absolute difference* (AD), *mean squared error* (MSE) and *standard deviation of absolute error* (SAE), as respectively defined in (5.2.4 – 5.2.6), are adhered. It is important to note that the predicted values (direct energy gradient value due to effective clogging, filter's global permeability, etc.) for each referenced experiment are derived from the specific model after its respective training step with the augmented training instances. The predicted values are then compared directly with the respective non-augmented dataset for the concerned parameters.

$$AD = \frac{1}{N} \sum_{i=1}^N |(Y_{pred,i} - Y_{obs,i})| \quad (5.2.4)$$

$$MSE = \frac{1}{N} \sum_{i=1}^N (Y_{pred,i} - Y_{obs,i})^2 \quad (5.2.5)$$

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$$SAE = \sqrt{\frac{1}{N} \sum_{i=1}^N \left(|Y_{pred,i} - Y_{obs,i}| - \frac{1}{N} \sum_{i=1}^N |Y_{pred,i} - Y_{obs,i}| \right)^2} \quad (5.2.6)$$

where $Y_{pred,i}$ is the model prediction value, and $Y_{obs,i}$ the actual measured value for the given indexing (i) of the non-augmented data points, and N the total number of data before augmentation.

Chapter 6: Experimental runs to simulate clogging conditions in depth filters

Chapter Overview:

This chapter describes additional experimental runs carried out in this thesis study for simulating the physical, chemical and biological clogging conditions taking place inside porous media (sand and carbon grains) column systems. The objective is to build up the pool of training instances to calibrate the proposed analytical (from Chapters 3 and 4) and numerical (from Chapter 5) models, which can subsequently be useful to achieve the predictive maintenance objective for operating depth filters on the industry scale.

Chapters 6.1, 6.2 and 6.3 respectively describe the experimental materials and methodology adopted for simulating the physical, chemical and biological clogging conditions taking place inside porous media column tests.

6.1. Experimental simulation of physical clogging conditions

Figure 6.1.1 illustrates an experimental sand column to remove emulated turbidity particles of varying bulk concentrations under constant-rate rapid filtration flow conditions. The turbidity particles influents were synthesized with PSP polyamide seeding particles (DANTEC, DYNAMICS) suspensions. For the sand column, the media was first washed thoroughly with tap water and dried in the oven at 100°C for a period of 24 hours to remove dust impurities. After drying, mechanical sieving was performed to obtain the effective size ($d_{c,0}$) of 0.2mm and uniformity coefficient (UC) of approximately 1.5. The column system has an inner-diameter size of 15cm and height of 125cm which is fully connected to built-in influent and effluent tanks of 440L in volume capacity as shown in Figure 6.1.1. 50cm of sand media was deployed for the rapid filtration experiments.

For every rapid filtration run, appropriate amounts of polyamide particles were added into the influent tank containing tap water and mixed thoroughly with an inline mixer to synthesize varying concentrations of monodisperse turbidity particles influents. Table 6.1.1 summarizes the varying experimental conditions carried out for each rapid filtration run. Note that a minimum d_p value of 20 μ m was maintained for the experiments to simulate the common particle size range for rapid filtration in

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seawater desalination facilities as a pre-treatment step. No additional pre-treatment was adopted for the synthesized suspensions due to the tendency of the polyamide particles to agglomerate easily.

Figure 6.1.1. Experimental rapid filter setup to simulate physical clogging of turbidity particles in sand column tests.

Table 6.1.1. Summary of experimental conditions carried out for each rapid filtration run to simulate physical clogging condition in sand filter.

Run	$V_s (m/h)$	$L_m (m)$	$d_g (mm)$	$c_0 (mg/L)$	$d_p (\mu m)$	$\rho_p (kg/m^3)$	$\mu_{in} (kg/ms)$	$t^* (h)$	t (throughput units)
1	6.0	0.5	0.20	157.6	50	1030	0.000860	1.5	18
2	6.0	0.5	0.20	136.0	50	1030	0.000860	2.0	24
3	6.0	0.5	0.20	172.2	50	1030	0.000860	2.0	24
4	6.0	0.5	0.20	151.0	20	1030	0.000860	1.5	18
5	6.0	0.5	0.20	127.0	20	1030	0.000860	1.5	18

Prior to start of each rapid filtration run, the sand filter was backwashed with tap water to ensure fully saturated conditions. The average background turbidity for Singapore's tap water was measured to be very low at around 0.17 NTU. Constant-rate rapid filtration mode of the sand column was maintained by manually adjusting an in-built flow valve regulator which recycled some influents back to its source tank (Figure 6.1.1). Temperature of the influent source was monitored consistently with a glass thermometer which was determined to remain constant at 27 °C - 28°C in all runs. Readings of the pressure gauge sensors at Locations 3, 4, 5, 6 and 7 were recorded after 5 seconds from the start of the experiment to serve as the clean filter

Chapter 6: Experimental runs to simulate clogging conditions in depth filters

pressure head values. Note that Location 2 did not record the fluid pressure as there is no media presence, since only 50cm of sand was adopted for the rapid filtration experiments.

At every 5-minute time interval, pressure head readings were again taken at the above-mentioned sampling locations to track the additional head loss incurred due to the simulated physical clogging condition inside the sand filter column. Samples were also collected from Location 7 for turbidity measurements with a portable Turbidimeter (2100N, HACH Company, USA) and for total suspended solids (*TSS*) measurements. Experimental measurements for turbidity and *TSS* parameters were in accordance to the Standard Methods for the Examination of Water and Wastewater (Standard Methods, 1960). All glassware materials used for sample collections were washed thoroughly with deionised water and dried before use. At the end of each filtration run, maintenance, via backwashing, was carried out for 10 minutes to restore the depth filter back to its original clean state before the next filtration run in Table 6.1.1. No air scouring was adopted for the backwashing process.

6.2. Experimental simulation of chemical clogging conditions

A series of adsorption experiments was carried out with the same lab-scale single-filter setup (Figure 6.1.1), as described in the previous sub-section, to simulate the chemical clogging condition in the experimental filter. Instead of sand, porous granular activated carbon (GAC) having the effective size (d_{10}) of 0.85mm and $> 1000m^2/g$ BET surface area was deployed for the column tests. 60cm of GAC media depth was instead deployed for each adsorption experiment. Likewise, the carbon grains were first washed thoroughly with tap water and dried in the oven at 100°C for 24 - 36 hours to remove any naturally occurring organic materials. The average total carbon organic (TOC) concentrations of the synthesized sub-microns natural organic matter (NOM) influents, which were prepared using concentrated humic acid solution together dechlorinated tap water, ranged closely between 10 to 15mg/L over the course of each experimental run as summarized in Table 6.2.1. Note that the NOM influents of the stated concentration values in the same table were prepared daily during each run.

Chapter 6: Experimental runs to simulate clogging conditions in depth filters

Table 6.2.1. Summary of experimental conditions carried out for each creeping flow filtration run to simulate chemical clogging condition in adsorbers.

Run	$V_s(\text{ml}/\text{min})$	$L_m(\text{m})$	$d_g(\text{mm})$	$c_0(\text{mg}/\text{L})$	$d_p(\mu\text{m})$	$\rho_p(\text{kg}/\text{m}^3)$	$\mu_{in}(\text{kg}/\text{ms})$	$t^*(\text{d})$	t (throughput units)
1	22.0	0.6	0.85	13.0 ± 2.0	$<<1$	1300	0.000860	14	41.8
2	25.0	0.6	0.85	11.8 ± 1.5	$<<1$	1300	0.000860	24	81.6
3	37.5	0.6	0.85	11.8 ± 1.5	$<<1$	1300	0.000860	11	56.1

During each run, 50ml of samples were collected daily at Location 8 for TOC measurements with a Total Organic Carbon Analyzer (ASI-V, Shimadzu). All glassware materials used for sample collections were washed thoroughly with deionised water and dried before use. Using a Masterflex peristaltic pump, the prepared NOM influents were transported from the influent tank to the top of the GAC column under creeping flow filtration conditions. Constant-flux, not constant-rate, filtration condition was maintained during the filtration runs. It was observed that negligible amounts of the prepared humic acid solution precipitated on the inner walls of the connected tubing during the runs.

Likewise, fully saturated conditions were ensured within the GAC column by flushing out the available airspace above the GAC media, via an installed air-valve at the top of the column, with dechlorinated tap water. Downward filtration of the prepared NOM influents was then initiated. The first TOC measurement for the effluent sample, collected from Location 8 in Figure 6.1.1, commenced 1 hour after the start of each filtration run which served as the initial (background) TOC value. Temperature of the influent source was again found to remain constant at 27 °C - 28°C in all filtration runs. Filter maintenance was carried out by replacing the original media with a new set of washed and dried carbon media before the start of the next experimental run in Table 6.2.1.

Chapter 7: Results and Discussions

Chapter Overview:

This chapter constitutes the core of this thesis work by discussing, in both quantitative and qualitative details, four key sub-sections, namely: (7.1) Supervised learning and validation of proposed theoretical models; (7.2) Validation of DRFM model; (7.3) Supervised learning and validation of RNN-LSTM model; and (7.4) Models applications for predictive maintenance objective.

Section 7.1 describes the different types of supervised learning methods, which include regression analysis, shallow deep fully connected neural network modelling, etc., adopted to calibrate the identified key parameters from the derived homogenized averaged representations for modelling the specific clogging condition in depth filter systems under creeping flow conditions. Appropriate validations, via time-series extrapolation means, of the calibrated parameters are then performed to test the model's capability for the predictive maintenance objective. Section 7.2 performs the model validation of DRFM, while Section 7.3 adopts suitable supervised learning methods to train and validate the predictive capabilities of RNN-LSTM tool for modelling the physical clogging condition in rapid depth filtration facilities. Upon appropriate verifications of the models' capabilities, extensive quantitative and qualitative details are provided in Section 7.4 to describe how the proposed models can be useful to field engineers to perform the predictive maintenance act of depth filters which undergo transient physical and chemical clogging conditions under varying flow conditions.

7.1. Supervised learning and validation of proposed theoretical models

7.1.1. Modelling physical clogging under creeping flow condition

Readers are referred to the published work of Chew and Law (2019a) for the full details of the proposed model built to quantify the complex physical clogging condition in depth filters under creeping flow condition. By first combining the homogenized averaged solution of (3.3.11) with dimensional analysis, (4.1.4) is shown to be the key quantitative representation to model the physical clogging condition in depth filters under creeping flow condition. A shallow deep multi-layered neural network (NN)

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model, as illustrated in Figure 7.1.1, is proposed to train (4.1.4) with an augmented pool of training instances derived from Section 4.1 previously.

Figure 7.1.1. Illustration of feature engineering step combined with dimensional analysis to build compacted input node for shallow deep multi-layered neural network (NN) architecture comprising of 4 hidden layers for supervised learning of physical clogging condition in depth filters.

The proposed NN model in Figure 7.1.1 is only based on trial and error and extensively varying the number of neurons in the different hidden layers is not performed for this study. Instead, the hyperparameters of learning rate, number of epochs and number of mini batches are varied accordingly with the model's training period, in terms of filter's throughput units (dimensionless term), to determine the most suitable combination of hyperparameters for the proposed NN model which can effectively analyse depth filter's physical clogging condition over time. For initializing the unknown weightages at each neuron in the hidden layers, Xavier Initialization algorithm is adopted as it maintains enough activation values and backpropagation gradients and can mitigate the exploding/vanishing problems during the network training. The rectified linear unit (ReLU) activation function is also attached to the neurons in the hidden layers as the function is expected to effectively predict time-valued outputs at each neuron during every epoch run using positive input features from (4.1.4) in this study.

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Direct simple regression analysis or least squares method is avoided for directly fitting the raw measured data for the $\ln(\tilde{k})$ parameter in (3.3.11) as the derived empirical equation does not link their calibrated coefficients to the known physical parameters associated with the filter's physical clogging condition. Extrapolation of the $\ln(\tilde{k})$ values in the measured data is not encouraged as there is no definite means to confirm that the fitted trend will continue for the extrapolated period. Rather, the proposed approach of combining the theoretical model with dimensional analysis is helpful to directly link the temporal variations of the $\ln(\tilde{k})$ to the key calibration coefficient within the homogenized representation, which is in turn associated to hybrid variations of the known physical parameters. Hence, the resulting engineering model can relate the hybrid variations of those parameters to the depth filters' breakthrough timings under creeping flow conditions for predictive maintenance objective. In addition, the model, having an optimized set of hyperparameters, enables us to fulfil the targeted objective by flexibly varying the pre-processed input layer and predict their hybrid effects on the filter's breakthrough timing due to the physical clogging condition taking place inside the filter at an early stage.

The following set of hyperparameters: (a) the learning rate (α_1) of values 0.01, 0.001 and 0.0001; (b) the sizes of mini-batches (α_2) of values of 4, 8 and 16; and (c) the number of epochs (α_3) of values 100, 300 and 500, are varied accordingly for the grid-search test by using the augmented measured data from Zhou et al. (2009) (Figure 4c in their paper) and Wang et al. (2012) (Figure 3b in their paper) respectively. For the latter component, only the augmented data from the authors' Figure 3b (Wang et al., 2012) is adhered to investigate the effects of varying the above-listed hyperparameters on the NN model's predictive capability. Note that the other measured data from the authors' Figures 3a and 3c (Wang et al., 2012) were previously derived from the same filter configuration in their study. Therefore, the optimized set of hyperparameters determined for that specific study should work for all measured data derived from the same filter setup (Figures 3a and 3c in their paper).

Using an initial 30% - 35% training period of the filter's total operational period in throughput units for the respective experiments (Zhou et al., 2009; Wang et al., 2012), 80% of the augmented training instances is adhered to investigate the variations of

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the above-listed hyperparameters. Note that the remaining 20% of the augmented training instances is used for validating the model's predictive accuracy for the same defined 30% - 35% training period. This procedure is part of the cross-validation step. Tables 7.1.1 and 7.1.2 list the respective root-mean-squared-error (RMSE) values derived from the comparison between NN model's predictions, using the calibrated weightages and biased term, and measured data (before data augmentation) from the entire training period (training plus cross-validation steps) for the respective experimental works of Zhou et al. (2009) (Figure 4c in their paper) and Wang et al. (2012) (Figure 3b in their paper). The combination of $\alpha_1 = 0.001$, $\alpha_2 = 4$ and $\alpha_3 = 300$ is determined to result in the lowest possible RMSE value as shown in Tables 7.1.1 and 7.1.2 respectively, which will then be adopted for further model training with other combinations of training periods in filter's throughput units. Note that RMSE is computed from the squared-root form of the MSE cost function as defined in (5.2.5).

For extensiveness, the training periods are further reduced to 10% and 20% of the filter's total operational period (in throughput units) in each referenced experiment (Zhou et al., 2009; Wang et al., 2012) which are then associated with the respective testing periods of 90% and 80% respectively. Tables 7.1.3 and 7.1.4 show that the RMSE values derived from the entire training step (training plus cross-validation steps), for the respective referenced experiments, gradually reduce with increasing training periods as expected. Too short of a training period (10% and 20%) results in high inaccuracies in the subsequent testing stages as shown in Tables 7.1.3 and 7.1.4. At present, the initial selected 30% to 35% training period is deemed most appropriate to maintain a balance between the computed RMSE from the later testing period and the need to predict the filter's breakthrough timing at a reasonably early stage of its operations. Large training period for effective model calibration may, however, deprive field engineers of the right amount of time to properly manage the predictive maintenance act in terms of the logistics and resources required.

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Table 7.1.1. Effects of varying learning rate (α_1), number of epochs (α_2) and size of mini-batches (α_3) on model's predictive accuracy for entire training step (training + cross-validation) using referenced experiment of Zhou et al. (2009) (Figure 4c in their paper).

Combination	α_1 (learning rate)	α_2 (sizes of mini batches)	α_3 (number of epochs)	RMSE (training)
1	0.01	4	100	0.249
2	0.001	4	100	0.249
3	0.0001	4	100	0.0302
4	0.01	8	100	0.249
5	0.001	8	100	0.249
6	0.0001	8	100	0.0300
7	0.01	16	100	0.249
8	0.001	16	100	0.0302
9	0.0001	16	100	0.0303
10	0.01	4	300	0.249
*11	0.001	4	300	0.0302
12	0.0001	4	300	0.0302
13	0.01	8	300	0.249
14	0.001	8	300	0.0302
15	0.0001	8	300	0.0303
16	0.01	16	300	0.249
17	0.001	16	300	0.0302
18	0.0001	16	300	0.0302
19	0.01	4	500	0.249
20	0.001	4	500	0.0302
21	0.0001	4	500	0.0302
22	0.01	8	500	0.249
23	0.001	8	500	0.0302
24	0.0001	8	500	0.0302
25	0.01	16	500	0.249
26	0.001	16	500	0.0302
27	0.0001	16	500	0.0302

*** lowest possible RMSE**

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Table 7.1.2. Effects of varying learning rate (α_1), number of epochs (α_2) and size of mini-batches (α_3) on model's predictive accuracy for entire training step (training + cross-validation) using referenced experiment of Wang et al. (2012) (Figure 3b in their paper).

Combination	α_1 (learning rate)	α_2 (sizes of mini batches)	α_3 (number of epochs)	RMSE (training)
1	0.01	4	100	0.134
2	0.001	4	100	1.14
3	0.0001	4	100	1.14
4	0.01	8	100	1.14
5	0.001	8	100	0.136
6	0.0001	8	100	1.14
7	0.01	16	100	0.0793
8	0.001	16	100	0.0805
9	0.0001	16	100	1.14
10	0.01	4	300	1.14
*11	0.001	4	300	0.0744
12	0.0001	4	300	1.14
13	0.01	8	300	1.14
14	0.001	8	300	0.0857
15	0.0001	8	300	1.14
16	0.01	16	300	1.14
17	0.001	16	300	1.14
18	0.0001	16	300	0.0998
19	0.01	4	500	1.14
20	0.001	4	500	1.14
21	0.0001	4	500	1.14
22	0.01	8	500	1.14
23	0.001	8	500	1.14
24	0.0001	8	500	1.14
25	0.01	16	500	1.14
26	0.001	16	500	1.14
27	0.0001	16	500	1.14

*** lowest possible RMSE**

Table 7.1.3. Effects of varying training periods on model's predictive accuracy for the entire training and testing steps using steps using augmented training instances from Zhou et al. (2009) (Figure 4c in their paper).

Training period (%)	RMSE (training step)	Testing period (%)	RMSE (testing step)
10	0.0351	90	0.742
20	0.0316	80	0.219
35	0.0302	65	0.170

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Table 7.1.4. Effects of varying training periods on model's predictive accuracy for the entire training and testing steps using steps using augmented training instances from Wang et al. (2012) (Figure 3b in their paper).

Training period (%)	RMSE (training step)	Testing period (%)	RMSE (testing step)
10	0.102	90	0.604
20	0.0812	80	0.499
35	0.0744	65	0.246

The optimized set of hyperparameters ($\alpha_1 = 0.001$, $\alpha_2 = 4$ and $\alpha_3 = 300$), as determined previously, is then adhered to further test the model's predictive accuracy for the remaining 65% to 70% of the filter's total operational period in the different referenced experiments (Zhou et al., 2009; Wang et al., 2012) as illustrated in Figures 7.1.2 to 7.1.5. Figure 7.1.2 shows reasonable agreement (average of 0.173 in RMSE value) between the model's predictions with the respective measured data (before data augmentation) (Zhou et al., 2009, Figure 4c in their paper). The unexpected jump in the measured values for $\ln(\tilde{k}(\varepsilon^{-1}, t))$ in the time range of $10 \leq t \leq 15$ in Figure 7.1.2 could be attributed to the sudden detachment of the initially trapped contaminants inside the experimental filter which then resulted in a spike in the filter's average global permeability as shown. To capture this sudden change to the permeability transient profile, the following changes can be made.

- Add in the additional detachment term to Equation (3.1.4) which has initially been neglected for modelling the filter's physical clogging behavior, and then repeat the same analytical steps for modelling the chemical clogging behavior.
- Maintain the same derivations for modelling the filter's physical clogging behavior while extending the training period to encapsulate a degree of the sudden change between the throughput units of 10 and 15.

On the contrary, the average RMSE values in Figures 7.1.3 to 7.1.5 (average of 0.242, 0.246 and 0.163 in RMSE values respectively) are generally higher than that of Figure 7.1.2 due to the stagnating tail-end which may be indicative of a dominant balance between the trapping and detachment rates of contaminants, hence leading to minimum transient changes to the filter's average global permeability. At present, this physical behaviour cannot be captured by the proposed feature engineering

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(analytical derivations, via engineering mechanics, coupled with dimensional analysis) in this study.

Figure 7.1.2. Comparison between measured and predicted values from NN model for $\ln(\tilde{k}(\epsilon^{-1}, t))$ parameter during training and testing stages for the referenced experiment of Zhou et al. (2009) (Figure 4c in their paper).

Figure 7.1.3. Comparison between measured and predicted values from NN model for $\ln(\tilde{k}(\epsilon^{-1}, t))$ parameter during training and testing stages for the referenced experiment of Wang et al. (2012) (Figure 3a in their paper).

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Figure 7.1.4. Comparison between measured and predicted values from NN model for $\ln(\tilde{k}(\epsilon^{-1}, t))$ parameter during training and testing stages for the referenced experiment of Wang et al. (2012) (Figure 3b in their paper).

Figure 7.1.5. Comparison between measured and predicted values from NN model for $\ln(\tilde{k}(\epsilon^{-1}, t))$ parameter during training and testing stages for the referenced experiment of Wang et al. (2012) (Figure 3c in their paper).

7.1.2. Modelling chemical clogging under creeping flow condition

Prior to the training step, k_{ads} in the modified form of β in (3.4.16) is expressed as follows:

$$k_{ads} = \frac{\alpha}{x_K'}, \quad (7.1.1)$$

where $\alpha = \frac{l}{L} \frac{\ln(c)U\left(\tilde{k}\frac{\partial p}{\partial x_K'}\right)}{(1-\theta)\left(1-\frac{[\sim O(1)](1-\gamma)\theta}{\gamma(1-\theta)}\right)}$ and is a positive quantity.

For simplicity, the seepage velocity term of $\left(\tilde{k}\frac{\partial p}{\partial x_K'}\right)$ in α of (7.1.1) is estimated as $-\frac{V_s}{\theta U}$ to compact the uncertainties of the unknowns into the calibration coefficients

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of n_1 and n_2 in (4.2.3). Note that $\frac{|S|}{|\Omega|_V}$ is assumed as $(1 - \theta)$ for approximating the dimensionless pore spaces occupied by the ideal spheres within each cell domain and $\sim O(1)$ in α represents the ordering of importance between k_{ads} and k_{des} which are both materializing complexly within the macroscale adsorber. Since $\ln(c)$ varies slowly over the phase-2 stage (Figures 4.2.1 and 4.2.2), k_{ads} will also change correspondingly during the same period due to the inherent complexity. Note that $\ln(c) < 0$ for c values less than the unity value at any given filter's throughput units.

To perform the analysis, we first split the total filter's throughput units of phase-2 stage from Figures 4.2.1 and 4.2.2 into the following combinations of training and testing periods: (a) first 10% for training and next 90% for testing; (b) first 20% for training and next 80% for testing; (c) first 30% for training and next 70% testing; and (d) first 50% for training and next 50% for testing. The objective is again to determine the optimal training period which can achieve the highest possible balance between the model's accuracy, derived from the combined training and testing steps, and the need to approximate the timing for the filter to reach its exhaustion stage at a reasonably early timing of phase-2 stage. Note that simple regression analysis, not deep shallow multi-layered NN modelling from the previous sub-section, is now adopted to model the chemical clogging condition occurring inside adsorbers.

The following procedures are carried out for each of the referenced experiment from Figures 4.2.1 and 4.2.2 for model training which is then followed by testing the model's predictive capability.

- i. For the pre-defined training period (10%, 20% 30% and 50% of the total phase-2 period in throughput units), adopt the associated augmented dataset for c from Section 4.2 to compute the raw values of k_{ads} from (7.1.1) at the maximum media depth. Note that the number of k_{ads} training instances should correspond to the size of the augmented data pool for c , i.e. 10000 in quantity in this thesis study.
- ii. Adopt the raw values of k_{ads} from step (i) to calibrate n_1 and n_2 based on the determined pi-terms from (4.2.3). For simplicity, n_1 is taken as the value of unity as the first approach.

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- iii. For each raw value of k_{ads} , there will be a unique n_2 calibrated value. Hence, there will also be 10000 in quantity for the calibrated n_2 values associated with each defined training period (10%, 20% 30% and 50% of the total phase-2 period) for each referenced experiment involved in model training.
- iv. Determine the average n_2 value from step (iii).
- v. Adopt the average value of n_2 from step (iv) to determine the respective k_{ads} from (4.2.3) for the defined training period (10%, 20% 30% and 50% of the total phase-2 period).
- vi. Adopt the average value of n_2 from step (iv) to determine the respective k_{ads} from (4.2.3) for the remaining testing period (50%, 70%, 80% and 90% of the total phase-2 period).
- vii. The computed k_{ads} values from step (vi) are then used to compute c from (3.4.16) for the associated testing period.
- viii. Compare predicted and measured values for c by evaluating the average RMSE values for the entire phase-2 stage (training plus testing steps) to check the model's predictive capability. Note that this step differs slightly from that of the physical clogging analysis in the previous sub-section.

By considering the maximum media depth, i.e. $x_K' = \varepsilon^{-1}$, Figure 7.1.6 compares the predicted and measured values for c in the entire phase-2 stage (training and testing steps) in throughput units for each of the referenced experiments by using 50% of the respective total phase-2 period in filter's throughput units for model training. Readers are referred to Appendix C for the remaining figure plots which compare the predicted and measured values for c in the entire phase-2 stage (training and testing steps) in throughput units for each of the referenced experiments by using other training periods (10%, 20% and 30%) for model training.

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Figure 7.1.6a. Comparison between measured and predicted values for c over varying throughput units from 50% training period of total phase-2 operational period from own experimental runs.

Figure 7.1.6b. Comparison between measured and predicted values for c over varying throughput units from 50% training period of total phase-2 operational period from referenced experiments of Treumann et al. (2014).

Figure 7.1.6c. Comparison between measured and predicted values for c over varying throughput units from 50% training period of total phase-2 operational period from referenced experiments of Zhao et al. (2016).

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Tables 7.1.5, 7.1.6 and 7.1.7 list the respective RMSE (squared root of MSE function defined in (5.2.5)) values for the combined training and testing steps with accordance to each varied training periods in the different referenced experiments. Note that the proposed predictive model is trained and validated respectively with the different sets of measured data. It is also worth noting that the RMSE values for the entire predictive range of the dataset are given for the respective referenced experiment (Tables 7.1.5 to 7.1.7) as it has been observed that the corresponding RMSE value for the training and testing (validation) stages did not differ significantly. Hence, the overall RMSE value will be a conservative choice of value for estimating the accuracy of the breakthrough time made by the predictive model for the chemical clogging analysis.

The approximated values for n_2 , k_{ads} and k_{des} in each experiment, calibrated using different training periods via regression analysis with respect to the above-mentioned steps (i – viii) for model training, are summarized in Table D (Appendix D). The obtained results generally indicate that too short of the training period will result in high inaccuracies in the predicted values as expected. At present, selecting 30% - 50% of the total phase-2 stage for model training results in an average RMSE value of 0.15 or less in all referenced experiments. In addition, the defined 30% - 50% training period is likely to be considered as sufficiently early for engineers to perform predictive maintenance of the operating adsorbers, based on the known physical parameters within the coupled form of (4.2.3) and (7.1.1). This observation aligns with the physical clogging analysis from the previous sub-section in determining the best possible training period to perform predictive maintenance of depth filters undergoing slow physical clogging over time.

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Table 7.1.5. Effects of varying training period on RMSE values for training + testing steps for entire phase-2 operational period of own experimental runs.

Training period	Run 1 (RMSE for training + testing)	Run 2 (RMSE for training + testing)	Run 3 (RMSE for training + testing)
10%	0.101	0.173	0.129
20%	0.0990	0.146	0.127
30%	0.0969	0.140	0.125
*50%	0.0908	0.135	0.124

*** lowest possible RMSE**

Table 7.1.6. Effects of varying training period on RMSE values for training + testing steps for entire phase-2 operational period from referenced experiments of Treumann et al. (2014).

Training period	Treumann et al. 2014 (Figure 4a) (RMSE for training + testing)	Treumann et al. 2014 (Figure 4b) (RMSE for training + testing)	Treumann et al. 2014 (Figure 4c) (RMSE for training + testing)
10%	0.270	0.0947	0.186
20%	0.217	0.0598	0.151
30%	0.147	0.0506	0.0975
*50%	0.0876	0.0554	0.112

*** lowest possible RMSE**

Table 7.1.7. Effects of varying training period on RMSE values for training + testing steps for entire phase-2 operational period from referenced experiments of Zhao et al. (2016).

Training period	Zhao et al. 2016 (Figure 4a) (RMSE for training + testing)	Zhao et al. 2016 (Figure 4b) (RMSE for training + testing)
10%	0.145	0.103
20%	0.127	0.107
30%	0.140	0.101
*50%	0.132	0.0936

*** lowest possible RMSE**

The predicted c values from the present model can only asymptotically approach the value of 1.0 over time as observed in Figure 7.1.6. Predicting values greater than 1.0 cannot be done at this stage which, however, is necessary for some cases whereby the measured c exceeds the unity value at certain filter's throughput units during operations. To address this current limitation and improve the present model's accuracy, we avoid pre-fixing n_1 as 1.0 during the entire phase-2 period. After step (v) in the above-mentioned procedures to calibrate k_{ads} during model training, we further minimise the average RMSE value, to the lowest possible extent, from the training step by calibrating a suitable n_1 . The estimated n_1 value is then used to predict c for the remaining testing stage. This new proposition is examined with the defined 50% training period for all referenced experiments whereby general improvements to the

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model's accuracy occur for all referenced experiments as expected (see Figure 7.1.7 and Table 7.1.8).

Figure 7.1.7a. Comparison between measured and predicted values for c over varying throughput units from 50% training period of total phase-2 operational period from own experimental runs by pre-calibrating n_1 value.

Figure 7.1.7b. Comparison between measured and predicted values for c over varying throughput units from 50% training period of total phase-2 operational period from referenced experiments of Treumann et al. (2014) by pre-calibrating n_1 value.

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Figure 7.1.7c. Comparison between measured and predicted values for c over varying throughput units from 50% training period of total phase-2 operational period from referenced experiments of Zhao et al. (2016) by pre-calibrating n_1 value.

Table 7.1.8. Summary of post-calibrated n_1 values from the optimal 50% training period of the entire phase-2 operational periods for the different referenced experiments.

Experiment	RMSE (new)	RMSE (original)	n_1
Present experiment (set 1)	0.0843	0.0907	0.674
Present experiment (set 2)	0.0969	0.135	0.755
Present experiment (set 3)	0.0860	0.124	0.539
Treumann et al., 2014 (Figure 4a)	0.0454	0.0876	0.216
Treumann et al., 2014 (Figure 4b)	0.0355	0.0554	0.001
Treumann et al., 2014 (Figure 4c)	0.0802	0.112	0.640
Zhao et al., 2016 (Figure 4a)	0.118	0.132	0.850
Zhao et al., 2016 (Figure 4b)	0.0800	0.0936	0.001

Closer inspections of the measured raw data from Figures 4.2.1 and 4.2.2 indicate periodic oscillations in the concentration parameter which cannot be captured by the present analysis by far. Hence, an alternative approach is again proposed by modelling k_{ads} as a periodic function which can be sinusoidal, cosine or a combination of both functions, i.e. Fourier series. If a periodic function fits the raw measured data well during the training step, then it becomes possible to estimate the periodic time cycle for the concentration variations in all referenced experiments. To investigate this proposition, the following steps are put forth by using 50% of the total phase-2 stage for model training.

- Without performing any data augmentation a priori, estimate the raw values of k_{ads} from the respective c values for the first 50% period of the total phase-2 stage by using (7.1.1).

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- ii. Assume the maximum k_{ads} ($k_{ads,max}$) from step (i) to calibrate the unknown periodic function (sinusoidal, cosine or Fourier series).
- iii. For each of the estimated k_{ads} value from step (i), compute the angular frequency w from the assumed periodic function. For example, if a sinusoidal function is assumed, the equation of $k_{ads} = k_{ads,max} \sin(wt)$ is adhered.
- iv. Assume the average w ($w_{average}$) value from step (iii).
- v. Adopt $k_{ads,max}$ and $w_{average}$ from steps (ii) and (iv) respectively to compute the range of k_{ads} values for the entire phase-2 stage (training plus testing steps).
- vi. The computed k_{ads} values from step (v) are then used to compute c from (3.4.16) for the entire phase-2 stage.
- vii. Compare the predicted values (derived from step (vi)) and the respective measured values for c by evaluating the average RMSE for the entire phase-2 period (training + testing) to evaluate the proposition of using periodic functions to quantify the oscillatory behaviour of the concentration parameter.

With respect to the raw measured data from Figures 4.2.1 and 4.2.2, either a sinusoidal or cosine periodic function is assumed to quantify the transient variations of k_{ads} in the above step (iii) for the respective referenced experiment. Figure 7.1.8 and Table 7.1.9 show that the proposed alternative approach results in further improvements to the agreement between the predicted and measured values for the concentration parameter. Note that no periodic function can be determined to fit the raw training instances for the referenced experiment of Zhao et al. (2012, Figure 4b in their paper).

In summary, the proposed introduction of the periodic function is based on the following reasonings: (a) linear characteristic of the dimensionless equation for k_{ads} in (4.2.3) does not capture the fluctuating concentration behavior as shown in Figures 7.1.6 to 7.1.8 in the predictions made from the trained model; and (b) visual inspections of the raw data in Figures 7.1.6 to 7.1.8 suggest that the concentration profile follows a near-periodic transient trend. The present assumption of the periodic function existence is based solely on inspecting the available raw data and can only be confirmed with extended runs of the respective experimental runs which cannot be achieved at this stage. In practice, the field engineer can determine the suitability of

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the periodic functions by first attempting the original approach of training the dimensionless equation for k_{ads} in (4.2.3) via supervised learning and evaluate if the resulting predictive accuracy from the testing (validation) stage is reasonable based on judgement and domain understanding.

Figure 7.1.8a. Comparison between measured and predicted values for c using 50% training period of total phase-2 operational period from own experiments by assuming a suitable periodic function for k_{ads} .

Figure 7.1.8b. Comparison between measured and predicted values for c using 50% training period of total phase-2 operational period from Treumann et al. (2014) by assuming a suitable periodic function for k_{ads} .

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Figure 7.1.8c. Comparison between measured and predicted values for c using 50% training period of total phase-2 operational period from Zhao et al. (2016) by assuming a suitable periodic function for k_{ads} .

Table 7.1.9. Summary of estimated w values by assuming a sinusoidal or cosine periodic function for k_{ads} from the optimal 50% training period of the entire phase-2 operational periods for the different referenced experiments.

Experiment	RMSE (new)	RMSE (original)	w	Type of periodic function
Own experiment (set 1)	0.0392	0.0843	0.0195	Cosine
Own experiment (set 2)	0.0905	0.0969	0.0386	Sinusoidal
Own experiment (set 2)	0.0827	0.0860	0.0232	Cosine
Treumann et al., 2014 (Figure 4a)	0.0593	0.0454	0.642	Sinusoidal
Treumann et al., 2014 (Figure 4b)	0.0358	0.0355	0.149	Sinusoidal
Treumann et al., 2014 (Figure 4c)	0.0819	0.0802	0.813	Sinusoidal
Zhao et al., 2016 (Figure 4a)	0.0927	0.118	2.15	Sinusoidal

7.2. Model validation of DRFM

Readers are referred to the published work of Chew and Law (2018a) for the full details of the proposed DRFM numerical model built to quantify the physical clogging condition in depth filters under rapid flow condition. Verification of DRFM's predictive capability is first performed accordingly with the adopted operating parameters in this study as listed in Table 6.1.1. Using (5.1.1), DRFM adopts a unique length scale parameter (θ'_A) to account for the surface area effects of the trapped turbidity particles on the rapid filter's direct energy gradient metric incurred over time $(\Delta H)_t$. Note again that θ'_A is based on an empirical relationship between the respective sizes of the collector grain and turbidity particle which are known a priori. Readers are referred to Appendix A for the exact quantitative details. Figures 7.2.1a to 7.2.1e demonstrate

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reasonably good agreement between the DRFM predictions and measured raw data for $(\Delta H)_t$ under varying operating conditions from Table 6.1.1. At present, the average RMSE value for the error deviations between the predictions and measurements for all 5 runs approximate to 0.0403, 0.0203, 0.0520, 0.0600 and 0.0410 respectively.

Figure 7.2.1a. Comparison between DRFM predictions and raw measured data for $(\Delta H)_t$ using Run 1 operating conditions from Table 6.1.1.

Figure 7.2.1b. Comparison between DRFM predictions and raw measured data for $(\Delta H)_t$ using Run 2 operating conditions from Table 6.1.1.

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Figure 7.2.1c. Comparison between DRFM predictions and raw measured data for $(\Delta H)_t$ using Run 3 operating conditions from Table 6.1.1.

Figure 7.2.1d. Comparison between DRFM predictions and raw measured data for $(\Delta H)_t$ using Run 4 operating conditions from Table 6.1.1.

Figure 7.2.1e. Comparison between DRFM predictions and raw measured data for $(\Delta H)_t$ using Run 5 operating conditions from Table 6.1.1.

The comparison results from Figure 7.2.1a to 7.2.1e indicate that DRFM can account for surface area effects of the trapped turbidity particles on $(\Delta H)_t$, which

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quantitative understanding remains limited by far. Hence, DRFM can be suitable to predict $(\Delta H)_t$ for any given combination of the intake feed conditions and the changing media characteristics within the rapid filter during its effective physical clogging stage. The good agreement obtained also suggests that DRFM can be useful to perform the predictive maintenance act of rapid filters which can provides long-term economies of scale benefit for field engineers, as demonstrated in later sections.

DRFM is also expected to be able to account for the inhomogeneous physical clogging effect along the filter's media depth as evident in Figures 7.2.2a to 7.2.2c, whereby the trapping of larger turbidity particles leads to larger grain diameters within the rapid filter's upper media compartments at its final throughput units. This is because larger particles have less tendency to penetrate deep into the filter which results in bulk volume of particles to be removed within the filter's uppermost regions. Note that the value of unity for $\frac{d_c}{d_0^*}$ corresponds to the original effective size of d_0^* at $\frac{z}{L_m} = 0$. In Figures 7.2.2d to 7.2.2e, DRFM instead predicts smaller spatial gradients for d_c in the regions of $\frac{z}{L_m} \leq 0.1$ which indicates a more homogeneous spatial distribution of the same mass volume of smaller turbidity particles trapped within the filter as smaller-sized particles have greater tendency to penetrate deeper.

Figure 7.2.2a. DRFM predictions of inhomogeneous clogging effect of media grains at filter's final throughput units for physical clogging of turbidity particles in Run 1 of Table 6.1.1.

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Figure 7.2.2b. DRFM predictions of inhomogeneous clogging effect of media grains at filter's final throughput units for physical clogging of turbidity particles in Run 2 of Table 6.1.1.

Figure 7.2.2c. DRFM predictions of inhomogeneous clogging effect of media grains at filter's final throughput units for physical clogging of turbidity particles in Run 3 of Table 6.1.1.

Figure 7.2.2d. DRFM predictions of inhomogeneous clogging effect of media grains at filter's final throughput units for physical clogging of turbidity particles in Run 4 of Table 6.1.1.

Figure 7.2.2e. DRFM predictions of inhomogeneous clogging effect of media grains at filter's final throughput units for physical clogging of turbidity particles in Run 3 of Table 6.1.1.

To further justify DRFM's capability to account for the inhomogeneous spatial clogging condition in depth filters, Figures 7.2.3a to 7.2.3c demonstrate larger reduction in the experimental filter's global porosity under effective clogging conditions (ϵ_c) at its final throughput units within the regions of $\frac{z}{L_m} \leq 0.05$ when trapping larger-sized turbidity particles. In contrast, the porosity reduction at the final throughput units is less significant in the same region when trapping smaller-sized particles as shown in Figures 7.2.3d to 7.2.3e. DRFM assumes the value of ϵ_0 at $\frac{z}{L_m} = 0$.

Figure 7.2.3a. DRFM predictions of inhomogeneous clogging effect of filter's global porosity at final throughput units for physical clogging of turbidity particles in Run 1 of Table 6.1.1.

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Figure 7.2.3b. DRFM predictions of inhomogeneous clogging effect of filter's global porosity at final throughput units for physical clogging of turbidity particles in Run 2 of Table 6.1.1.

Figure 7.2.3c. DRFM predictions of inhomogeneous clogging effect of filter's global porosity at final throughput units for physical clogging of turbidity particles in Run 3 of Table 6.1.1.

Figure 7.2.3d. DRFM predictions of inhomogeneous clogging effect of filter's global porosity at final throughput units for physical clogging of turbidity particles in Run 4 of Table 6.1.1.

Figure 7.2.3e. DRFM predictions of inhomogeneous clogging effect of filter's global porosity at final throughput units for physical clogging of turbidity particles in Run 3 of Table 6.1.1.

The above results indicate that DRFM can model rapid filters' clogging dynamics for any given combination of operating parameters (controlled and non-controlled) with the following resulting outcomes.

- Establish the filter's effective filtration stage by accounting for the appropriate particle removal mechanisms
- Demonstrate in quantitative details the inhomogeneous physical clogging effects on the media diameters and filter's global porosity along the media depth
- Sufficiently accurate predictions of filter's direct energy gradient metric due to effective physical clogging conditions for contributing to the predictive maintenance objective

7.3. Supervised learning and validation of RNN-LSTM model

As discussed previously, RNN-LSTM aims to improve on DRFM's predictive accuracy for modelling rapid filters' direct energy gradient incurred during their effective physical clogging stages. DRFM mainly differs from RNN-LSTM by requiring an initial learning phase of the filter's direct energy gradient transient profile, i.e. $(\Delta H)_t$, with respect to the augmented pool of training instances derived in Section 5.2. Using the operating conditions of Runs 1 to 3 in Table 6.1.1, the training periods of 10%, 20% and 30% of the respective filter's total throughput units are adopted to train RNN-LSTM with two augmented datasets of 500 (Data-1) and 1000 (Data-2) in quantities in each run.

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Tables 7.3.1a and 7.3.1b list the optimal set of hyperparameters for Data-1 and Data-2 augmented datasets respectively which can best minimize mean-squared-error (MSE) as the selected cost function for RNN-LSTM's predictions associated with the combined training and testing steps in Runs 1 to 3 (from Table 6.1.1) as discussed in Section 5.2.

Table 7.3.1a. Optimal sets of hyper-parameters (number of epochs, batch size, learning rate) required to train RNN-LSTM for Runs 1 to 3 from Table 6.1.1 with varying training periods using Data-1 augmented dataset.

Run	Number of epochs	Batch size	Learning rate	MSE
1 (10% training period)	150	8	0.001	0.000334
*1 (20% training period)	150	32	0.1	0.000316
1 (30% training period)	50	4	0.001	0.000962
2 (10% training period)	50	2	0.001	0.00118
2 (20% training period)	150	16	0.001	0.00141
*2 (30% training period)	100	32	0.001	0.000224
3 (10% training period)	100	1	0.001	0.00189
*3 (20% training period)	50	8	0.001	0.000851
3 (30% training period)	100	32	0.001	0.00103

Table 7.3.1b. Optimal sets of hyper-parameters (number of epochs, batch size, learning rate) required to train RNN-LSTM for Runs 1 to 3 from Table 6.1.1 with varying training periods using Data-2 augmented dataset.

Run	Number of epochs	Batch size	Learning rate	MSE
*1 (10% training period)	50	4	0.001	0.000386
1 (20% training period)	100	8	0.001	0.000413
1 (30% training period)	150	16	0.001	0.00110
2 (10% training period)	100	16	0.001	0.00106
*2 (20% training period)	100	32	0.001	0.000227
2(30% training period)	50	16	0.001	0.000844
3 (10% training period)	150	4	0.001	0.00224
3 (20% training period)	150	2	0.001	0.000525
*3 (30% training period)	100	32	0.001	0.000183

*** lowest possible MSE**

Considering both Data-1 and Data-2 augmented datasets, Figures 7.3.1 to 7.3.3 compare the measured (non-augmented dataset) and predicted $(\Delta H)_t$ values from RNN-LSTM for the experimental filter's transient direct energy gradient incurred during its effective clogging stage associated with each of the different training periods (10%, 20% and 30%) respectively. Tables 7.3.1a (Data-1) and 7.3.1b (Data-2) respectively list the average values of the computed AD (Equation 5.2.4), MSE (selected cost

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function from Equation 5.2.5 for model training) and SAE (Equation 5.2.6) metrics for comparing the measured (non-augmented dataset) and predicted $(\Delta H)_t$ values from RNN-LSTM in Runs 1 to 3 from Table 6.1.1.

The following key observations for Runs 1 to 3 from Table 6.1.1 can be derived from the simulation results of RNN-LSTM.

- DRFM generally over-predicts the filter's direct energy gradient over time as building towards its breakthrough stage, i.e. filter's direct energy gradient value at a specific time exceeds the defined threshold value, as shown for Runs 1 and 3 in Figures 7.3.1 and 7.3.3 respectively.
- RNN-LSTM better captures the experimental filter's long-term behavior for its direct energy gradient metric as building towards the defined breakthrough stage in Runs 1 and 3 (Figures 7.3.1 and 7.3.3). This may be most useful as field engineers will usually perform maintenance (backwashing) based on the filter's direct energy gradient value incurred at a later operational timing.
- DRFM predicts better than RNN-LSTM in Run 2 in Figure 7.3.2 based on the average AD value computed using the total number of non-augmented data points.
- Predictions made by RNN-LSTM in using Data-1 and Data-2 augmented datasets are sufficiently close, as shown in the computed average values of AD, MSE and SAE in Tables 7.3.1a (Data-1) and 7.3.1b (Data-2). Hence, the selected sizes of the augmented datasets (Data-1 and Data-2) are currently reasonable to ensure convergence in the transient direct energy gradient values computed. As such, further augmenting the sizes of the respective raw datasets is not necessary to enhance the predictive accuracy of RNN-LSTM in Runs 1 to 3 from Table 6.1.1.
- Using different quantities of the augmented dataset (Data-1 and Data-2), the optimal training period will vary accordingly for training RNN-LSTM in each of the respective runs. Refer to Tables 7.3.1a (Data-1) and 7.3.1b (Data-2) for the different optimal training periods determined for the respective runs based on their average MSE values computed.

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- The average error deviation, based on the AD metric, between the measured (non-augmented dataset) and predicted direct energy gradient values from RNN-LSTM ranges between 0.0100 and 0.0200 for the respective optimal training periods determined for Runs 1 to 3 using Data-1 (Table 7.3.1a) and Data-2 (Table 7.3.1b).

Figure 7.3.1a. Comparison between RNN-LSTM (using Data-1 and Data-2 augmented datasets) and DRFM predictions, by using 10% of the respective total operational period as training period, with measured data derived from Run 1 in Table 6.1.1.

Figure 7.3.1b. Comparison between RNN-LSTM (using Data-1 and Data-2 augmented datasets) and DRFM predictions, by using 10% of the respective total operational period as training period, with measured data derived from Run 2 in Table 6.1.1.

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Figure 7.3.1c. Comparison between RNN-LSTM (using Data-1 and Data-2 augmented datasets) and DRFM predictions, by using 10% of the respective total operational period as training period, with measured data derived from Run 3 in Table 6.1.1.

Figure 7.3.2a. Comparison between RNN-LSTM (using Data-1 and Data-2 augmented datasets) and DRFM predictions, by using 20% of the respective total operational period as training period, with measured data derived from Run 1 in Table 6.1.1.

Figure 7.3.2b. Comparison between RNN-LSTM (using Data-1 and Data-2 augmented datasets) and DRFM predictions, by using 20% of the respective total operational period as training period, with measured data derived from Run 2 in Table 6.1.1.

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Figure 7.3.2c. Comparison between RNN-LSTM (using Data-1 and Data-2 augmented datasets) and DRFM predictions, by using 20% of the respective total operational period as training period, with measured data derived from Run 3 in Table 6.1.1.

Figure 7.3.3a. Comparison between RNN-LSTM (using Data-1 and Data-2 augmented datasets) and DRFM predictions, by using 30% of the respective total operational period as training period, with measured data derived from Run 1 in Table 6.1.1.

Figure 7.3.3b. Comparison between RNN-LSTM (using Data-1 and Data-2 augmented datasets) and DRFM predictions, by using 30% of the respective total operational period as training period, with measured data derived from Run 2 in Table 6.1.1.

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Figure 7.3.3c. Comparison between RNN-LSTM (using Data-1 and Data-2 augmented datasets) and DRFM predictions, by using 30% of the respective total operational period as training period, with measured data derived from Run 3 in Table 6.1.1.

At present, DRFM from the preceding sub-section cannot handle the following situations for modelling rapid filters' direct energy gradient over time during its effective physical clogging stage.

- Sudden detachment of the initially trapped turbidity particles within the depth filter which can cause the filter's direct energy gradient values to fluctuate over time.
- Filtering influents of high polydispersivity, i.e. multiple particle sizes within the suspensions, which complicates the computations of the filter's direct energy gradient values over time.

RNN-LSTM is, however, expected to better account for the above-conditions due to the prior model training step. DRFM currently computes the filter's direct energy gradient development rate using only its initial known physical parameters and works well only if the filter's effective filtration stage is well-maintained during its operations. Specifically, it means that DRFM still assumes that the media grains grow continuously over time due to constant particles deposition, leading to a concurrent rise in the filter's direct energy gradient over time. Effective filtration can, however, be affected by the sudden detachment of the trapped particles from the filter which then affects its global porosity. A drop in the porosity value will then increase the filter's initial permeability which then slows down its direct energy gradient development rate during the clogging phase. Quite often, detachment can be detected by engineers via either a quick rise in the effluent's turbidity value recorded or a slowdown in the sensor readings of the

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fluid pressure inside the filter. The former scenario is most difficult to handle a priori as the filters must usually stop operations upon detections which then leads to unexpected logistical problems.

Supervised training of RNN-LSTM with measured data can be useful to encapsulate a degree of the real-world complexity associated with the rapid filter's online operations. For example, if detachment of particles occurs during the defined training period, then RNN-LSTM can capture the complex behavior and model its effects on the filter's direct energy gradient during the extrapolation step as building towards its breakthrough stage. Even for scenarios whereby the detachment behavior is not captured within the defined training period, engineers can still extend the period, via trial and error during batch (offline) model training, to determine the new training period which can better model the particle detachment effect on the filter's direct energy gradient incurred over time.

RNN-LSTM's predictive capability is further examined with a more varied range of experimental conditions (concentration of influents, particle size etc.) from previous studies (Darby et al., 1992; Veerapaneni and Wiesner., 1993; Hunt et al., 1993; Han et al., 2009) as summarized as new Runs 1 to 4 respectively in Table 7.3.2. Likewise, the same data augmentation procedures and training algorithms are adopted to model the new experimental conditions. No augmented dataset is used for model training in the new Run 3 experiment in Table 7.3.2 as the proposed data interpolation method did not work well for the model training step in that run, in terms of the resulting accuracy derived from the combined training and testing steps. Hence, the original dataset (approximately 255 training instances) in Run 3 from Table 7.3.2 is maintained for the model training step.

Table 7.3.2. Summary of additional experimental conditions adopted to test RNN-LSTM predictive capability.

Run	$V_s(m/h)$	$L_m(m)$	$d_g(mm)$	$c_0(mg/L)$	$d_p(\mu m)$	$\rho_p(kg/m^3)$	$\mu(kg/ms)$	$t(h)$	t (throughput units)
1	6.12	0.09	0.55	12.6	0.6	1050	0.000900	4.18	284
2	4.75	0.135	0.364	6.54	0.944	1300	0.000970	5.01	176
3	10.0	0.320	1.29	30.0	30	2420	0.00114	3.5	109
4	5.0	0.900	0.500	2.40	3.00	1400	0.00152	28.6	159

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The optimal set of hyperparameters required for model training with the operating conditions of the new Runs 1 to 4 from Table 7.3.2 with varying training periods are summarized in Tables 7.3.3a and 7.3.3b. Again, the predictions from RNN-LSTM of the filter's direct energy gradient metric for new Runs 1 and 2 (see Figures 7.3.4 and 7.3.5 respectively) are very close for both Data-1 and Data-2 augmented datasets in the respective figures. On the contrary, the latter dataset size results in lower AD, MSE, SAE metrics, i.e. higher predictive accuracy, for the new Run 4 as shown in Figure 7.3.6. At present, RNN-LSTM can predict the direct energy gradient of any arbitrary rapid filter over time with reasonable accuracy due to the prior model training step which encapsulates a degree of the real-world complexity inherent to any filter configuration (lab-, pilot-, industrial-scales etc.).

One concern from the present analysis is that RNN-LSTM requires 50% of the total operational time (in terms of filter's total throughput units) for relative effective model training as shown in Figures 7.3.6 and 7.3.7 respectively. Generally, a longer training period implies that operators have less amount of time to manage the logistics and resources required for filter maintenance. The need for longer training periods in Figures 7.3.6 and 7.3.7 could be ascribed to the following reasons: (a) some environmental externalities/factors when operating the experimental or pilot-scale filters have not been captured by RNN-LSTM, i.e. there may be other important input features to be identified for modelling the filter's direct energy gradient cost over time; and (b) relatively low quality in the raw dataset, especially for Figure 7.3.7 whereby there are consistent transient fluctuations in the filter's direct energy gradient values as extracted from the literature. Therefore, a more effective data-cleaning step may be helpful prior to training RNN-LSTM, particularly for the simulation run associated with Figure 7.3.6.

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Table 7.3.3a. Optimal sets of hyper-parameters (number of epochs, batch size, learning rate) required to train RNN-LSTM for the new Runs 1 to 4 from Table 7.3.2 with varying training periods using Data-1 augmented dataset.

Run	Number of epochs	Batch size	Learning rate	MSE
1 (10% training period)	100	32	0.001	0.131
1 (20% training period)	50	1	0.01	0.0519
*1 (30% training period)	50	8	0.001	0.00149
2 (10% training period)	50	8	0.001	0.00266
2 (20% training period)	100	8	0.001	0.00318
*2 (30% training period)	50	16	0.001	0.00254
3 (10% training period)	100	32	0.001	0.780
3 (20% training period)	150	1	0.001	0.134
3 (30% training period)	100	2	0.001	0.0737
*3 (50% training period)	50	32	0.001	0.0529
4 (10% training period)	50	32	0.001	0.654
4 (20% training period)	50	32	0.001	0.653
4 (30% training period)	100	16	0.01	0.592
*4 (50% training period)	100	16	0.01	0.0220

*** lowest possible MSE**

Table 7.3.3b. Optimal sets of hyper-parameters (number of epochs, batch size, learning rate) required to train RNN-LSTM for the new Runs 1 to 4 from Table 7.3.2 with varying training periods using Data-2 augmented dataset.

Run	Number of epochs	Batch size	Learning rate	MSE
1 (10% training period)	100	32	0.001	0.212
1 (20% training period)	100	2	0.001	0.0107
*1 (30% training period)	50	32	0.001	0.00144
2 (10% training period)	100	32	0.001	0.00189
2 (20% training period)	50	32	0.001	0.00186
*2 (30% training period)	50	32	0.001	0.00281
3 (10% training period)	100	32	0.001	0.780
3 (20% training period)	150	1	0.001	0.134
3 (30% training period)	100	2	0.001	0.0737
*3 (50% training period)	50	32	0.001	0.0529
4 (10% training period)	50	32	0.001	0.705
4 (20% training period)	50	32	0.001	0.690
4 (30% training period)	100	16	0.01	0.0291
*4 (50% training period)	150	16	0.001	0.0388

*** lowest possible MSE**

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Figure 7.3.4. Comparison between RNN-LSTM (using Data-1 and Data-2 augmented datasets) and DRFM predictions, by using 30% of the respective total operational period as training period, with measured data derived from new Run 1 in Table 7.3.2.

Figure 7.3.5. Comparison between RNN-LSTM (using Data-1 and Data-2 augmented datasets) and DRFM predictions, by using 30% of the respective total operational period as training period, with measured data derived from new Run 2 in Table 7.3.2.

Figure 7.3.6. Comparison between RNN-LSTM (using Data-1 and Data-2 augmented datasets) and DRFM predictions, by using 50% of the respective total operational period as training period, with measured data derived from new Run 3 in Table 7.3.2.

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Figure 7.3.7. Comparison between RNN-LSTM (using Data-1 and Data-2 augmented datasets) and DRFM predictions, by using 50% of the respective total operational period as training period, with measured data derived from new Run 4 in Table 7.3.2.

In addition, simple regression analysis is also performed for the new Runs 1 to 4 (as shown in Figures 7.3.4 to 7.3.7 respectively) to justify that using deep learning methods in RNN-LSTM will not result in an overkill situation when modelling rapid filters' direct energy gradient metric during their effective physical clogging stages. Tables 7.3.4a (Data-1) and 7.3.4b (Data-2) list the most suitable type of polynomial equations for the new Runs 1 to 4 which result in the highest possible accuracies for the entire training and testing steps by using the previously determined optimal training period for each run from Tables 7.3.3a (Data-1) and 7.3.3b (Data-2). Presently, the first-order linear representation is determined to be most suitable for the fitting analysis of the operating conditions associated with the new Runs 1 to 4 from Table 7.3.2. The calibrated weightages and biased term for the respective linear regression models used in the new Runs 1 to 4 with Data-1 and Data-2 are summarized in Tables 7.3.5a and 7.3.5b for reference. The two tables indicate that both Data-1 and Data-2 result in very similar values for the calibrated coefficients pertaining to the regression model, hence confirming that convergence in the model predictions has been attained. In addition, Figures 7.3.4 to 7.3.6 also show that the predictions from the regression model are near-identical from the use of Data-1 and Data-2 augmented datasets.

Again, the accuracies provided by the regression model are generally lower than that of RNN-LSTM as summarized in Tables 7.3.4a and 7.3.4b for both Data-1 and Data-2 datasets. Overall, the amount of time invested, i.e. longer periods of model training, in fine-tuning the inherent hyperparameters of RNN-LSTM is effective to

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ensure the improved accuracy of its predictions as demonstrated in this study. Note that the pre-processed input layer is identical for the different approaches (regression model and RNN-LSTM), hence the coupled RNN and LSTM algorithms is likely to be responsible for the observed difference in the RNN-LSTM final predictions as compared to that of the simple regression models. By performing enough number of iterations to determine the optimal sets of hyperparameters, it thus becomes possible for the forest gate within the LSTM cells (hidden layers) to determine the most important information, associated with the pre-processed input layer, to be stored for predictions in the long term by RNN-LSTM.

Tables 7.3.4a. Comparison of computed AD, MSE and SAE values derived from RNN-LSTM with Simple Regression Analysis for the new Runs 1 to 4 from Table 7.3.2 with optimal training periods using Data-1 augmented dataset.

Run	RNN-LSTM			Simple Regression Analysis			
	<i>AD</i>	<i>MSE</i>	<i>SAE</i>	<i>AD</i>	<i>MSE</i>	<i>SAE</i>	Type of polynomial representation
1 (30% training period)	0.0303	0.00149	0.0239	0.0569	0.00494	0.194	Linear
2 (30% training period)	0.0338	0.00254	0.0374	0.0358	0.00319	0.0437	Linear
3 (50% training period)	0.153	0.0529	0.137	0.294	0.114	0.156	Linear
4 (50% training period)	0.125	0.0220	0.0803	0.309	0.137	0.203	Linear

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Tables 7.3.4b. Comparison of computed AD, MSE and SAE values derived from RNN-LSTM with Simple Regression Analysis for the new Runs 1 to 4 from Table 7.3.2 with optimal training periods using Data-2 augmented dataset.

Run	RNN-LSTM			Simple Regression Analysis			
	<i>AD</i>	<i>MSE</i>	<i>SAE</i>	<i>AD</i>	<i>MSE</i>	<i>SAE</i>	Type of polynomial representation
1 (30% training period)	0.0285	0.00144	0.0251	0.0565	0.00489	0.0412	Linear
2 (30% training period)	0.0338	0.00281	0.0408	0.0358	0.00321	0.0438	Linear
3 (50% training period)	0.153	0.0529	0.137	0.294	0.114	0.156	Linear
4 (50% training period)	0.166	0.0388	0.106	0.309	0.137	0.203	Linear

Tables 7.3.5a. List of calibrated coefficients (weightages and biased terms) for either linear or quadratic polynomial representations in Simple Regression Analysis for the new Runs 1 to 4 from Table 7.3.2 using optimal training periods and Data-1 augmented dataset.

Run	Weightage for first-order feature	Weightage for second-order feature	<i>C</i>	Type of polynomial representation
1 (30% training period)	1.49	Nil	≈ 0	Linear
2 (30% training period)	0.348	Nil	≈ 0	Linear
3 (50% training period)	2.48	Nil	0.0656	Linear
4 (50% training period)	1.47	Nil	0.0237	Linear

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Tables 7.3.5b. List of calibrated coefficients (weightages and biased terms) for either linear or quadratic polynomial representations in Simple Regression Analysis for the new Runs 1 to 4 from Table 7.3.2 using optimal training periods and Data-2 augmented dataset.

Run	Weightage for first-order feature	Weightage for second-order feature	C	Type of polynomial representation
1 (30% training period)	1.49	Nil	≈ 0	Linear
2 (30% training period)	0.348	Nil	≈ 0	Linear
3 (50% training period)	2.48	Nil	0.0656	Linear
4 (50% training period)	1.47	Nil	0.0237	Linear

7.4. Models' application for predictive maintenance objective

7.4.1. Predictive maintenance for filters undergoing physical clogging behavior under creeping and rapid flow conditions

Starting with the physical clogging behavior under creeping flow condition, the proposed NN model from Section 7.1 is adopted to examine the effects of varying influent's concentration (c_0), average size of contaminants (d_p) and filter's hydraulic loading rate (V_s) on the filter's breakthrough timing (t_b) for maintenance purposes. For this scenario, t_b occurs when the filter's global permeability coefficient at its maximum media depth, i.e. $\ln(\tilde{k}(\varepsilon^{-1}, t))$, reaches its stagnation zone whereby there is likely to be a dominant balance between the removal and detachment rate of the contaminants inside the depth filter under creeping flow conditions as discussed previously. Two unique classes of parameters variations are carried out, namely: (a) varying uncontrollable parameters in both c_0 and d_p ; and (b) varying the controllable parameter in V_s . To demonstrate the usefulness of proposed approach, the physical filter parameters (Wang et al., 2012, Figure 3c in their paper) from Figure 7.1.5, due to its highest accuracy obtained from NN model, are adopted to simulate the above-listed parameters variations. For the former, Table 7.4.1 lists the predicted t_b values

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with accordance to each varied combination of c_0 and d_p for filtering both low- and high-concentration influents.

Tables 7.4.1. Summary of predicted timings from the NN model for filter configuration of (Wang et al., 2012, Figure 3c in their paper) to reach its breakthrough stage under varying c_0 and d_p values for maintenance.

Combination	$c_0(kg/m^3)$	$d_p (\mu m)$	$t_b (h)$	Preparatory time (h)
1	0.100	10	~ 9	~ 6
2	0.100	20	~ 18	~ 12
3	0.100	30	~ 27	~ 18
4	0.100	40	~ 36	~ 24
5	0.100	50	~ 44	~ 30
6	0.100	60	~ 54	~ 36
7	0.100	70	~ 62	~ 40
8	0.100	80	~ 72	~ 50
9	0.100	90	~ 81	~ 54
10	0.100	100	~ 90	~60
11	0.001	10	~ 900	~ 600
12	0.001	20	~ 1800	~ 1200
13	0.001	30	~ 2700	~ 1800
14	0.001	40	~ 3500	~ 2400
15	0.001	50	~ 4500	~ 3000
16	0.001	60	~ 5400	~ 3600
17	0.001	70	~ 6300	~ 4000
18	0.001	80	~ 7200	~ 4800
19	0.001	90	~ 8000	~ 5400
20	0.001	100	~ 9000	~ 6000

Tables 7.4.1 and 7.4.2 also list the amount of preparatory timings for each varied combination of the physical parameters based on a 30% initial training period for calibrating the proposed NN model as demonstrated in Section 7.1. Generally, the simulation results from Table 7.4.1 indicate close weightages to the effects contributed by $\frac{c_0}{\rho_p}$ and $\frac{L_m}{d_p}$ from (4.1.4), whereby higher c_0 and lower d_p values result in faster filter's breakthrough rate, i.e. smaller t_b values, as expected. Table 7.4.2 indicates that filtering high c_0 results in smaller t_b values for all V_s combinations which confirms that c_0 is relatively more influential than V_s in affecting t_b . On the contrary, the effects of V_s are more significant when filtering low c_0 by resulting in lower t_b as listed in Table 7.4.2. In summary, the trained NN model, with a reasonable early training period, can be useful for field engineers to predict the timing for any arbitrary depth filter to reach its breakthrough stage under creeping flow conditions, as based on the hybrid

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combinations of the physical parameters in (4.1.4). By doing so, significant amount of preparatory time is provided to field engineers, after the initial model training phase, to efficiently manage the logistics and resources required for filter maintenance.

Tables 7.4.2. Summary of predicted timings from the NN model for filter configuration of (Wang et al., 2012, Figure 3c in their paper) to reach its breakthrough stage under varying V_s values for maintenance.

Combination	$c_0(kg/m^3)$	$d_p(\mu m)$	$V_s(m/h)$	$t_b(h)$	Preparatory time (h)
1	0.100	50	0.200	~44	~30
2	0.100	50	0.210	~42	~28
3	0.100	50	0.220	~40	~27
4	0.100	50	0.230	~40	~27
5	0.100	50	0.240	~38	~25
6	0.100	50	0.250	~36	~24
7	0.100	50	0.260	~34	~23
8	0.100	50	0.270	~33	~22
9	0.100	50	0.280	~32	~21
10	0.100	50	0.290	~31	~20
11	0.100	50	0.300	~30	~20
12	0.001	50	0.200	~4400	~3000
13	0.001	50	0.210	~4300	~2900
14	0.001	50	0.220	~4200	~2800
15	0.001	50	0.230	~4100	~2800
16	0.001	50	0.240	~4000	~2700
17	0.001	50	0.250	~3900	~2600
18	0.001	50	0.260	~3900	~2600
19	0.001	50	0.270	~3800	~2500
20	0.001	50	0.280	~3700	~2500
21	0.001	50	0.290	~3700	~2500

Proceeding to the physical clogging behaviour under rapid flow conditions, both DRFM and RNN-LSTM can be adopted accordingly to demonstrate their advantages for the predictive maintenance act. Since RNN-LSTM generally performs better than DRFM in predicting rapid filters' direct energy gradient, the emphasis will be to describe the former's capabilities to garner long-term energy savings and greenhouse gases (GHG) reduction from the filters' predictive maintenance act. Readers are referred to the published work of Chew and Law. (2018) which thoroughly describes the advantages provided by DRFM for the predictive maintenance purpose of both single- and dual-media filter facilities. The former type remains popular in major desalination plants, as in the example of Tampa Bay (Tampa, 2018) which at around 44 million gallons per day (MGD).

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To demonstrate the advantages provided by RNN-LSTM for the predictive maintenance act of large-scale single-media filter facilities, the operating conditions of the new Run 4 from Table 7.3.2 are adopted since they were extracted from an actual water treatment plant in Yorkshire (Han et al., 2009, Figure 6 in their paper). The filter facility analyzed in that study had a cross-sectional area of $11m^2$. The parameters of V_s , c_0 and d_p are again varied in the following respective ranges: (a) $5.0m/h \leq V_s \leq 10.0m/h$; (b) $2.40mg/L \leq c_0 \leq 100.0mg/L$; and (c) $3.00\mu m \leq d_p \leq 50.0\mu m$, for the effective rapid filtration of both low- and high-turbid influents over time. All other parameters from Run 4 in Table 7.3.2 are kept unchanged.

The same trained RNN-LSTM model for the concerned run is maintained to simulate each combination of the above-perturbed operating parameters for the filter's direct energy gradient temporal profile. A total of 252 simulation runs is carried out for a total filtration period of 144 hours (6 operational days), which converts to 800 throughput units (Han et al., 2009, Figure 6 in their paper) in total from Table 7.3.2, to demonstrate the energy savings advantage quantitatively. For simulated runs which have not attained the breakthrough stage within 144 hours, the breakthrough time of 144 hours is then presumed for those runs to demonstrate the energy savings principle. The following additional assumptions are also made to perform the energy cost analysis:

- Maximum measured head loss due to effective clogging for operating the depth filter in the water treatment plant in Yorkshire was around 0.23m (Han et al., 2009, Figure 6 in their paper), which correlate to a value of 2.3 for $(\Delta H)_t$ with respect to Figure 7.3.7 in this analysis.
- Direct filtration energy cost thus approximates to $0.226 kWh/m^3$ from the preceding pointer and the listed operating conditions for Run 4 in Table 7.3.2.
- Backwashing (filter maintenance) will be initiated when $(\Delta H)_t$ reaches the value of 2.3 approximately.
- 100% recovery rate from the operating depth filters.

There are presently no reported values for the direct and indirect energy costs incurred for the actual depth filtration operations and treatment of the generated backwash waste in the case of Yorkshire (Han et al., 2009, Figure 6 in their paper).

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Hence, the following common assumptions, as extracted from relevant literature, are adhered for the respective energy costs to perform the cost analysis for the rapid filters' predictive maintenance act.

- Each backwash cycle will last about 30 minutes on average based on current industrial standards and typically consume about 4% of the total volume of filtrate produced a priori (Crittenden et al., 2012; Voutchkov, 2012, 2017a), which then also constitute to the same volume of backwash waste produced.
- Direct energy cost to treat the total volume of backwash waste, prior to de-watering, incineration and disposal, approximates to $0.270 \text{ kwh}/\text{m}^3$ (Voutchkov, 2012, 2017a).
- Average cost (indirect energy cost) for producing chemicals to treat total volume of backwash waste approximates to $\text{USD}0.05/\text{m}^3$ (Voutchkov, 2012, 2017a).
- Average electricity cost in UK's context approximates to $\text{USD}0.220/\text{Kwh}$ at present.

Figures 7.4.1a, 7.4.1b and 7.4.1c illustrate how the variations of c_0 and d_p , with respect to (5.2.3), affect the filter's breakthrough time (for maintenance) for the varying hydraulic loading rates of 5.0m/h, 7.5m/h and 10.0m/h respectively. Note that the 'X' representation in the x-axes of Figures 7.4.1a, 7.4.1b and 7.4.1c refers to the compacted form of (5.2.3) having C_2 as unity value. In summary, the following useful indicators can be made from those figures.

- Operate the depth filter at higher loading rates for extended periods, i.e. beyond the conventional 24 or 48h maintenance time-mark, prior to the breakthrough phase, to achieve economies of scale (EOS) when treating low-turbid influents (less than 40mg/L) having larger particles suspensions.
- For treating low-turbid influents of small particles suspensions, it is most conservative to operate the filter at lower loading rates for the possibility of extended operational runs to achieve EOS. The same conclusion can be made for the treatment of high-turbid influents (more than 40mg/L) of larger particles suspensions.
- Not possible to achieve EOS in any means for the treatment of high-turbid influents (more than 40mg/L) of smaller particles suspensions.

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Figure 7.4.1a. Predictions of rapid filter's breakthrough time (t_b), based on predictive maintenance act, using simulated perturbed operating parameters from new Run 4 in Table 6.2.3 at 5.0m/h hydraulic loading rate. 'X' represents the compacted form of (5.2.3).

Figure 7.4.1b. Predictions of rapid filter's breakthrough time (t_b), based on predictive maintenance act, using simulated perturbed operating parameters from new Run 4 in Table 7.2.3 at 7.5m/h hydraulic loading rate. 'X' represents the compacted form of (5.2.3).

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Figure 7.4.1c. Predictions of rapid filter's breakthrough time (t_b), based on predictive maintenance act, using simulated perturbed operating parameters from new Run 4 in Table 7.2.3 at 10.0m/h hydraulic loading rate. 'X' represents the compacted form of (5.2.3).

To compute the energy savings for each simulation run, the following scenarios are termed as follows: (S1) backwashing (filter maintenance) is carried out at every 24h; and (S2) backwashing at the optimal maintenance time as S2. Note that the volume of filtrate required for backwashing is identical in both S1 and S2 which approximates to 4% of the total filtrate produced at the 24h mark (Crittenden et al., 2012; Voutchkov, 2012, 2017a). (4.1) is then adhered to compute the respective E_{total} values, which is the total energy cost to treat per unit volume of filtrate (E_{total} , USD/ m^3) produced, for both S1 and S2 in all simulations runs.

$$E_{total} = \frac{\left[\left(0.270 \frac{kWh}{m^3} \times V_b \times \frac{USD0.220}{Kwh} \right) + \left(\frac{USD0.05}{m^3} \times V_b \right) + \left(\frac{USD0.220}{Kwh} \times E_t \times V_f \right) \right]}{V_f}, \quad (7.4.1)$$

where V_b and V_f are the volumes (m^3) of the backwash waste and filtrate produced respectively, and E_t is computed as follows.

$$E_t = \rho_s g [(\Delta H)_t + 1] H_0 \times 10^{-3} \quad (7.4.2)$$

where E_t (kWh/m^3) is the average kilowatt-hour required to effectively filter per unit m^3 of influent, and ρ_s the density of the influent being filtered.

The energy savings ($E_{savings}$, %) gained from the difference between S1 and S2 with respect to S1 as follows:

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$$E_{savings}(\%) = \frac{E_{total,S1} - E_{total,S2}}{E_{total,S1}} \times 100\%, \quad (7.4.3)$$

where $E_{total,S1}$ and $E_{total,S2}$ are the total energy costs to treat per unit volume of filtrate in S1 and S2 scenarios respectively.

Figures 7.4.2a to 7.4.2c illustrate the effects of varying c_0 and d_p on $E_{savings}(\%)$ for the varying hydraulic loading rates of 5.0m/h, 7.5m/h and 10.0m/h respectively. Generally, the figures show that the predictive maintenance act can result in both positive and negative $E_{savings}(\%)$ as depending on the different combinations of V_s , c_0 and d_p for the same filter configuration from Run 4 in Table 7.3.2. Hence, there is a need to determine an optimal balance among the simulated ranges of values for V_s , c_0 and d_p as demonstrated earlier too. Specifically, Tables 7.4.3a to 7.4.3c list the 10 random combinations of c_0 and d_p under varying hydraulic loading rates (5.0m/h, 7.5m/h and 10.0m/h) which can result in positive $E_{savings}(\%)$ as shown. The results also show that positive $E_{savings}(\%)$ can be achieved by optimal maintenance timings which vary across the different combinations of V_s , c_0 and d_p , and those timings can be higher or lower (in some cases) than the 24h or 48h maintenance time-mark presently adopted on the industrial scale.

Figure 7.4.2a. Predictions of rapid filter's energy savings (%), based on predictive maintenance act, using simulated perturbed operating parameters from new Run 4 in Table 6.2.3 at 5.0m/h hydraulic loading rate. 'X' represents the compacted form of (5.2.3).

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Figure 7.4.2b. Predictions of rapid filter's energy savings (%), based on predictive maintenance act, using simulated perturbed operating parameters from new Run 4 in Table 6.2.3 at 5.0m/h hydraulic loading rate. 'X' represents the compacted form of (5.2.3).

Figure 7.4.2c. Predictions of rapid filter's energy savings (%), based on predictive maintenance act, using simulated perturbed operating parameters from new Run 4 in Table 6.2.3 at 5.0m/h hydraulic loading rate. 'X' represents the compacted form of (5.2.3).

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Tables 7.4.3a. Summary of predicted energy savings (%) and annual energy savings (USD) from RNN-LSTM, based on predictive maintenance act, for simulated perturbed operating parameters from Run 4 in Table 7.3.2 at 5.0m/h hydraulic loading rate.

$d_p(\mu m)$	$c_0(mg/L)$	$t_b(h)$	$E_{savings}(\%)$ from operations in S2 relative to S1	Annual energy savings (USD) from operations in S2 relative to S1	$V_b(m^3)$ in S1	Annual energy savings (USD) from sludge treatment with incineration in S2 relative to S1	Annual energy savings (USD) from sludge treatment without incineration in S2 relative to S1
15	2.4	144	6.20%	11,900,000	317	4,740,000	10,200,000
30	2.4	144	6.20%	11,900,000	317	4,740,000	10,200,000
50	10	130	5.72%	10,900,000	286	4,160,000	8,950,000
45	10	117	5.26%	10,000,000	257	3,620,000	7,790,000
40	10	104	4.80%	9,090,000	229	3,080,000	6,620,000
35	10	91	4.33%	8,160,000	200	2,540,000	5,460,000
15	5	78	3.84%	7,200,000	172	2,000,000	4,300,000
30	10	78	3.84%	7,200,000	172	2,000,000	4,300,000
50	20	65	3.33%	6,230,000	143	1,460,000	3,130,000
45	20	59	3.09%	5,760,000	130	1,210,000	2,600,000

Tables 7.4.3b. Summary of predicted energy savings (%) and annual energy savings (USD) from RNN-LSTM, based on predictive maintenance act, for simulated perturbed operating parameters from Run 4 in Table 7.3.2 at 7.5m/h hydraulic loading rate.

$d_p(\mu m)$	$c_0(mg/L)$	$t_b(h)$	$E_{savings}(\%)$ from operations in S2 relative to S1	Annual energy savings (USD) from operations in S2 relative to S1	$V_b(m^3)$ in S1	Annual energy savings (USD) from sludge treatment with incineration in S2 relative to S1	Annual energy savings (USD) from sludge treatment without incineration in S2 relative to S1
30	2.4	144	6.20%	11,900,000	475	7,120,000	15,300,000
35	2.4	144	6.20%	11,900,000	475	7,120,000	15,300,000
40	5	139	6.03%	11,600,000	459	6,810,000	14,600,000
35	5	121	5.40%	10,300,000	399	5,680,000	12,200,000
15	2.4	108	4.94%	9,380,000	356	4,870,000	10,500,000
30	5	104	4.80%	9,090,000	343	4,620,000	9,930,000
50	10	87	4.18%	7,870,000	287	3,560,000	7,650,000
45	10	78	3.84%	7,210,000	257	3,000,625	6,440,000
40	10	70	3.53%	6,610,000	231	2,500,000	5,370,000
35	10	61	3.17%	5,920,000	201	1,940,000	4,160,000

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Tables 7.4.3c. Summary of predicted energy savings (%) and annual energy savings (USD) from RNN-LSTM, based on predictive maintenance act, for simulated perturbed operating parameters from Run 4 in Table 7.3.2 at 10.0m/h hydraulic loading rate.

$d_p(\mu m)$	$c_0(mg/L)$	$t_b(h)$	$E_{savings}(\%)$ from operations in S2 relative to S1	Annual energy savings (USD) from operations in S2 relative to S1	$V_b(m^3)$ in S1	Annual energy savings (USD) from sludge treatment with incineration in S2 relative to S1	Annual energy savings (USD) from sludge treatment without incineration in S2 relative to S1
30	2.4	144	6.20%	11,900,000	634	9,490,000	20,400,000
35	2.4	144	6.20%	11,900,000	634	9,490,000	20,400,000
40	2.4	144	6.20%	11,900,000	634	9,490,000	20,400,000
45	2.4	144	6.20%	11,900,000	634	9,490,000	20,400,000
50	2.4	144	6.20%	11,900,000	634	9,490,000	20,400,000
50	5	130	5.72%	10,900,000	572	8,330,000	17,900,000
45	5	117	5.26%	10,000,000	515	7,240,000	15,600,000
40	5	104	4.80%	9,090,000	458	6,160,000	13,200,000
35	5	91	4.33%	8,160,000	400	5,080,000	10,900,000
15	2.4	81	3.95%	7,430,000	356	4,250,000	9,130,000

The computed positive $E_{savings}(\%)$ values from Tables 7.4.3a to 7.4.3c can be converted into monetary gains for water-related infrastructures as demonstrated by a real-world example in the following. At present, the Yorkshire Water Utility Company is supplying potable water to more than 2.3 million households in Yorkshire. Each household in the UK consumes around $164m^3$ per year on average (Hoekstra and Chapagain, 2006). Hence, the total annual energy savings, in terms of monetary value (USD), derived from the predictive maintenance act for a large number of operating depth filters can be very significant in the case of Yorkshire, as summarized in Tables 7.4.3a to 7.4.3c, by using the total annual filtrate demand volume of approximately $377 \times 10^6 m^3$. The simulation results underline the usefulness of RNN-LSTM to achieve long-term energy savings from the operations of existing large-scale filter facilities via the predictive maintenance act as demonstrated quantitatively. By maintaining the same volume of filtrate (from S1) for backwashing the clogged filter in S2, engineers can also eliminate the unnecessary wastage of filtrate due to the reduction in the number of backwashing cycles, while ensuring extended production rate from the depth filters to provide EOS as discussed.

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The total volume of backwash sludge/waste produced from the filter maintenance process can either be discharged directly, without treatment, to sewage system or is treated and recycled within the plant (Edzwald, 2010). For the former scenario, significant energy savings can again be derived by reducing the volume of sludge produced from the predictive maintenance act. Based on previous studies (Mizuta and Shimada, 2010; Gu et al., 2017), the average energy costs to treat sewage sludge with and without incineration approximate to $0.935kWh/m^3$ and $2.01kWh/m^3$ respectively. Likewise, the proposed S1 and S2 scenarios are adopted to estimate the total annual energy savings gained from S2 case relative to that of S1.

For S2, filter maintenance is performed just once at the predicted t_b values, as shown in Tables 5a to 5c, whereas the maintenance frequency for S1 is estimated as $int(\frac{t_b}{24h})$ which directly result in the estimated volumes of backwash waste (Tables 7.4.3a to 7.4.3c) generated from the additional cycles of backwashing carried out in S1. Consequently, the total energy costs for sludge treatment with and without incineration in S1 will generally be higher, as compared to S2, in Tables 7.4.3a to 7.4.3c with respect to the total annual filtrate demand volumes required for Yorkshire's households. In addition, the obtained simulation results indicate a threshold maintenance timing (filter's breakthrough time) of around 30 hours in the case of Yorkshire which ensure a net annual energy savings, derived from the operating depth filters, in S2 relative to S1. In summary, extending the production rate of filtrate from the operating filters is effective to provide long-term net energy savings for both the operational and sludge treatment stages, particularly for large-scale filter facilities.

Generally, treatment of the backwash sludge can generate GHG gases, specifically carbon dioxide, methane and nitrous oxide as measured in carbon dioxide equivalents (CO_{2eq}). Reducing the volumes of sludge generated during the maintenance phase of the operating filters can be particularly useful to control the quantities of GHG gases produced during the treatment phase of the sludge (on-site or after transfer to the sewage treatment plants), particularly for operating large-scale filter facilities. Sludge contains turbidity particles and other contaminants removed within the depth filters, during their initial operational phase, and chemicals used for the prior coagulation and flocculation steps. Thus, the following specific treatment steps must be performed to

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handle properly handle the backwash sludge before appropriate disposal or incineration.

- Solids separation from backwash sludge
- Precipitation of chemicals used for prior coagulation and flocculation steps
- Increasing in oxygen content
- pH adjustment

The above-mentioned treatment steps contribute to the GHG gases generations during the sludge treatment step. Coupled with incineration, the total volume of GHG gases produced will increase due to additional volumes of nitrous oxide produced (Piippo et al., 2018). Typically, the average volume of nitrous oxide gases generated during the incineration step amounts to $1.46kgCO_{2eq}/m^3$ of sludge volumes treated in model sewage treatment plants which deploy rapid sand filters for post-treatment phase (Masuda et al., 2018). In addition, the average mass of carbon dioxide produced per unit mass of sludge (defined also as active substance) treated with polymers approximate to $2.62kgCO_{2eq}/kg_{active\ substance}$ (INCOPA, 2014; Parravicini et al., 2016) for thickening and dewatering processes. Accounting for these quantitative numbers and assuming a typical wet sludge of $1400kg/m^3$, we compute the mass of GHG gases produced, as measured in carbon dioxide equivalents in (7.4.4), in both S1 and S2 scenarios for the case of Yorkshire.

$$M_{GHG} = \left[\left(\frac{2.62kgCO_{2eq}}{kg_{active\ substance}} \times \left(\frac{1400kg}{m^3} \times V_b \right) \right) + \left(\frac{1.46kgCO_{2eq}}{m^3_{active\ substance}} \times V_b \right) \right], \quad (7.4.4)$$

The following expression is adopted to approximate the mass reduction of GHG gases ($M_{GHG,savings}$) in S2 relative to S1.

$$M_{GHG,savings} = M_{GHG,S2} \times \left(\frac{V_{b,S2}}{V_{b,S1}} \right), \quad (7.4.5)$$

where $M_{GHG,S2}$ is the mass of GHG generated in S2 scenario as measured in carbon dioxide equivalent, $V_{b,S1}$ and $V_{b,S2}$ represent the volumes of the backwash sludge/waste produced in S1 and S2 scenarios respectively.

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Likewise, the simulation results for M_{GHG} in Tables 7.4.4a to 7.4.4c again indicate that the operating filters in Yorkshire should approximately operate for at least 30h, prior to maintenance, to ensure a net reduction in M_{GHG} for S2 relative to S1 during the sludge treatment phase for the varied sets of V_s , c_0 and d_p conditions simulated. In summary, the above analysis shows that the minimum operating period of 30h will be necessary for the large-scale filter facilities in Yorkshire which can ensure both net annual energy savings and GHG reduction, as measured in monetary value and carbon dioxide equivalent respectively, from the operational and maintenance phases.

Tables 7.4.4a. Summary of mass of GHG gases reduction from RNN-LSTM, based on predictive maintenance act, for existing filters using simulated perturbed operating parameters from Run 4 in Table 7.3.2 at 5.0m/h hydraulic loading rate.

$d_p(\mu m)$	$c_0(mg/L)$	$t_b(h)$	$V_b(m^3)$ in S1	Annual $M_{GHG,savings}(kgCO_{2eq})$ savings in S2 relative to S1
15	2.4	144	317	9.22×10^9
30	2.4	144	317	9.22×10^9
50	10	130	286	1.02×10^{10}
45	10	117	257	1.14×10^{10}
40	10	104	229	1.28×10^{10}
35	10	91	200	1.46×10^{10}
15	5	78	172	1.70×10^{10}
30	10	78	172	1.70×10^{10}
50	20	65	143	2.04×10^{10}
45	20	59	130	2.25×10^{10}

Tables 7.4.4b. Summary of mass of GHG gases reduction from RNN-LSTM, based on predictive maintenance act, for existing filters using simulated perturbed operating parameters from Run 4 in Table 7.3.2 at 7.5m/h hydraulic loading rate.

$d_p(\mu m)$	$c_0(mg/L)$	$t_b(h)$	$V_b(m^3)$ in S1	Annual $M_{GHG,savings}(kgCO_{2eq})$ savings in S2 relative to S1
30	2.4	144	475	9.22×10^9
35	2.4	144	475	9.22×10^9
40	5	139	459	9.22×10^9
35	5	121	399	1.10×10^{10}
15	2.4	108	356	1.23×10^{10}
30	5	104	343	1.28×10^{10}
50	10	87	287	1.53×10^{10}
45	10	78	257	1.70×10^{10}
40	10	70	231	1.90×10^{10}
35	10	61	201	2.18×10^{10}

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Tables 7.4.4c. Summary of mass of GHG gases reduction from RNN-LSTM, based on predictive maintenance act, for existing filters using simulated perturbed operating parameters from Run 4 in Table 7.3.2 at 10.0m/h hydraulic loading rate.

$d_p(\mu m)$	$c_0(mg/L)$	$t_b(h)$	$V_b(m^3)$ in S1	Annual $M_{GHG,savings}(kgCO_{2eq})$ savings in S2 relative to S1
30	2.4	144	634	9.22×10^9
35	2.4	144	634	9.22×10^9
40	2.4	144	634	9.22×10^9
45	2.4	144	634	9.22×10^9
50	2.4	144	634	9.22×10^9
50	5	130	572	1.02×10^{10}
45	5	117	515	1.14×10^{10}
40	5	104	458	1.28×10^{10}
35	5	91	400	1.46×10^{10}
15	2.4	81	356	1.64×10^{10}

7.4.2. Predictive maintenance for filters undergoing chemical clogging behavior under creeping flow conditions

Building upon Section 7.1.2, the proposed predictive tool to model the chemical clogging condition in depth filters is leveraged by compacting (4.2.3) and (7.1.1) at the maximum media depth ($x_K' = \varepsilon^{-1}$) into the following form:

$$n_1 \left(\frac{d_p}{d_0^*} \cdot \rho_p A_g d_0^* \cdot \frac{c_0}{\rho_p} \cdot \frac{t^* V_s}{d_0^*} \cdot \frac{L_m}{d_0^*} \cdot \frac{d_0^* V_s}{v} \right)^{n_2} V_s = \frac{l}{L} \alpha, \quad (7.4.6)$$

From (7.4.6), the dimensional time parameter can be expressed as follows with appropriate manipulations.

$$t^* = \left(\frac{1}{n_1} \frac{l}{LV_s} \alpha \right)^{\frac{1}{n_2}} \left(\frac{d_p}{d_0^*} \cdot \rho_p A_g d_0^* \cdot \frac{c_0}{\rho_p} \cdot \frac{V_s}{d_0^*} \cdot \frac{L_m}{d_0^*} \cdot \frac{d_0^* V_s}{v} \right)^{-1}, \quad (7.4.7)$$

(7.4.7) provides the flexibility to vary any combinations of the known physical parameters to maximise a concerned adsorber's operational period before its exhaustion stage occurs for the maintenance act. For conservativeness, the breakthrough c value approximates to the value of 0.995 which is close to the exhaustion phase of $c \geq 1.0$. Retaining the calibrated n_2 values from the 50% training period for the experimental runs carried out in this thesis study (Figure 7.1.7a), the respective estimated t^* values to reach the limiting c values of 0.900, 0.950, 0.990,

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0.995 and 0.999 are summarized in Table 7.4.5. Note that the values in Table 7.4.5 have been converted into throughput units for convenience. With (5.6), engineers are thus provided with a predictive tool, built upon machine learning principles, to quickly estimate the timing for a concerned adsorber to asymptotically approach a limiting c value (as building towards to the exhaustion stage) for any given combination of the physical parameters. Hence, enough time is assured to minimize any possible logistical problems arising during the adsorber's operations, as discussed earlier.

Table 7.4.5. Summary of estimated throughput units for adsorber setup from Section 6.2 to reach different limiting c values by using (7.4.7)

Experiment	$c = 0.900$	$c = 0.950$	$c = 0.990$	$c = 0.995$	$c = 0.999$
Present experiment (set 1)	14.3	22.6	63.8	99.4	277.2
Present experiment (set 2)	22.4	36.0	105	166	474
Present experiment (set 3)	43.2	69.5	204	323	936

Building upon the use of periodic functions from Section 7.2, an alternative quantitative expression can be derived in (7.4.8) to improve on the timings for a concerned adsorber to reach different limiting c values of 0.900, 0.950, 0.990, 0.995 and 0.999 at the maximum media depth of $x_K' = \varepsilon^{-1}$. Table 7.4.6 summarizes the newly estimated t values for the adsorption experiments, as carried out in this study, with respect to the various limiting c values. Note that the new t values in Table 7.4.6 appeared to be more realistic as compared to that of Table 7.4.5, hence suggesting that using periodic functions will be most appropriate to encapsulate the complexity of the concurrent adsorption-desorption processes taking place in phase-2 stage.

$$t = \frac{\left\{ \begin{array}{l} \sin^{-1} \\ \cos^{-1} \end{array} \left(-\varepsilon^2 \frac{\ln(c) \left(\frac{V_s}{\Theta} \right)}{k_{ads,max} (1 - \Theta) \left(1 - \frac{[\sim O(1)] (1 - \gamma) \theta}{\gamma (1 - \theta)} \right)} \right) \right\}}{w}, \quad (7.4.8)$$

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Table 7.4.6. Summary of estimated throughput units for adsorber setup from Section 6.2 to reach different limiting c values by using (7.4.8)

Experiment	$c = 0.900$	$c = 0.950$	$c = 0.990$	$c = 0.995$	$c = 0.999$
Present experiment (set 1)	67.5	79.6	88.3	89.4	90.2
Present experiment (set 2)	51.8	56.6	60.3	60.7	61.1
Present experiment (set 3)	53.2	66.2	75.4	76.5	77.4

Chapter 8: Conclusion and future works

This chapter is divided into two key components. The first component summarizes the focus and key results derived from the present thesis study. The second component focuses on developing averaged homogenized representations, on a preliminary stage, to quantify the complex biological clogging in granular depth filters under creeping flow conditions for building towards the predictive maintenance objective as described in the previous Chapters. Following which, improvements to the proposed quantitative models are put forth which may better quantify the transient biological clogging behavior in filters.

Section 8.1 summarizes the completed works done in this thesis study. Section 8.2 is further divided into five sub-sections in the following format: (a) Section 8.2.1 describes the underlying mechanics responsible for the biological clogging condition taking place inside depth filters; (b) Section 8.2.2 homogenizes the first principle equations from Section 8.2.1; (c) Section 8.2.3 then describes the additional pre-processing steps undertaken to modify the homogenized representations as derived from the preceding Section; (d) Section 8.2.4 describes the experimental details involved to simulate the biological clogging condition in depth filters; (e) Section 8.2.5 performs the model training and validation step; and (f) Section 8.2.6 proposes the possible improvements to the models which may better quantify the complex biological clogging behavior inside depth filters for the predictive maintenance objective.

8.1. Conclusion of completed works

In summary, this thesis study focuses on building novel engineering models which can quantify the complex clogging behavior, of physical and chemical characteristics, in granular depth filters for the predictive maintenance objective. Different ranges of filtration velocities are considered, namely: (a) creeping flow condition whereby the microscale filtration Reynolds number is very much smaller than the value of unity; and (b) rapid flow condition having the same defined Reynolds number greater than the value of unity. Scenario (a) is modelled for the physical and chemical clogging behavior in mainly aquifer recharge and recovery systems (ARRS) settings, while scenario (b) is modelled for the physical clogging condition in rapid depth filters which

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are commonly deployed in water treatment and desalination facilities as post- and pre-treatment steps respectively.

For scenario (a), this thesis study innovates on the traditional homogenization theory coupled with the multiscale perturbation analysis to develop new homogenized averaged representations (theoretical models) which quantify the dynamics of the respective clogging condition over space and time. Unlike from previous studies, the present analysis adopts the averaged representations as an alternative feature extraction tool for supervised learning purpose. The objective is to reduce the feature space of the original high-dimensional clogging problem (physical and chemical characteristics) to accommodate for the current data-deficiency scenario. Specifically, each averaged representation for the different clogging condition contains a unique coefficient which is then modelled via dimensional analysis, as a function of the common physical parameters as described extensively in Chapter 4. Note that the values of those parameters will vary across different filter configurations.

Regression analysis, shallow-deep neural network modelling and long-short-term-memory neural network modelling are then carried out with training instances extracted from the literature and present study for training the proposed predictive models, derived by combining the homogenized representations with dimensional analysis, having the refined feature space from the common physical parameters. By far, reasonably good agreement is attained between the measured data and model's predictions for modelling each clogging condition in depth filters from the model training and validation steps. Quantitative and qualitative details are subsequently provided to demonstrate how the proposed models are leveraged to perform the predictive maintenance of depth filters undergoing the different clogging behavior over time.

In scenario (b), two different numerical models, termed as dynamical rapid filtration model (DRFM) and recurrent neural network coupled with long-short-term-memory (RNN-LSTM), are built to quantify the direct energy cost incurred by rapid filters during their effective physical clogging stage. Unlike from scenario (a), the pre-processed input layers of DRFM and RNN-LSTM are developed upon fundamental dimensional analysis, via the Buckingham pi-group theorem, of the commonly reported physical

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parameters which are expected to affect rapid filters' direct energy cost incurred during effective physical clogging. DRFM avoids using supervised learning methods for model training as it is based upon the physical representations which accounts for the growth rate of the media grains during the filter's clogging stage and how the growth rate affects the filter's direct energy cost computations using the known physical parameters. On the contrary, RNN-LSTM adopts a fair amount of training instances, as extracted from the literature and present study, for model calibration via supervised learning and then validated for its predictive accuracy. RNN-LSTM generally performs better than DRFM for modelling the direct energy gradient data. Subsequently, the capability of RNN-LSTM is demonstrated for the predictive maintenance act to derive long-term energy savings and GHG reduction for large-scale filter facilities with a real-world example.

8.2. Modelling biological clogging condition in depth filters

8.2.1. Mechanics responsible for biological clogging condition

Contaminants and microbes (of specific species) are expected to be present inside the fluid phase of any biofilter system. Fundamentally, both materials are again transported, via advection and diffusion, inside the fluid phase of the defined periodic cell domain as described in (8.2.1) and (8.2.2) respectively.

$$\frac{\partial c_m^*}{\partial t^*} + \frac{\partial(c_m^* u_i^*)}{\partial x_i^*} = \frac{\partial}{\partial x_i^*} \cdot \left(D_m^* \frac{\partial c_m^*}{\partial x_i^*} \right), \quad x^* \subset \Omega_f \quad (8.2.1)$$

$$\frac{\partial c_p^*}{\partial t^*} + \frac{\partial(c_p^* u_i^*)}{\partial x_i^*} = \frac{\partial}{\partial x_i^*} \cdot \left(D_p^* \frac{\partial c_p^*}{\partial x_i^*} \right), \quad x^* \subset \Omega_f \quad (8.2.2)$$

where the concentrations, c_m^* and c_p^* are the respective masses of microbes and contaminants per unit volume of fluid, D_m^* and D_p^* respectively represent the unknown diffusivity coefficients responsible for the transport of microbes and contaminants inside the fluid phase. Both D_m^* and D_p^* are affected by the respective molecular diffusion of microbes and contaminants, and the zig-zag trajectories inherent to the randomly packed media inside the biofilter.

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The complexity of the biofilm matrix within a real-world biofilter system is modelled by an idealized growth rate of a thin material layer, i.e. biofilm layer, around each media grain, which is similar to the theoretical idealization made for modelling the physical clogging condition in depth filters as defined in (3.1.7) previously. At the fluid-biofilm interface (Ω_{fB}), (8.2.3) accounts for the microbes undergoing an assumed first-order attachment process, due to the diffusion mechanism, from the fluid phase to the biofilm's boundary.

$$-\frac{\frac{\partial S_1^*}{\partial x_i^*}}{|\nabla S_1^*|} \cdot \left(D_m^* \frac{\partial c_m^*}{\partial x_i^*} \right) = k_{m,fb} c_m^*, \quad x^* \subset \Omega_{fB} \quad (8.2.3)$$

where S_1^* is the boundary of the biofilm layer with $\frac{\partial S_1^*}{\partial x_i^*}$ being its outward normal vector, and $k_{m,fb}$ the unknown attachment rate of microbes, having the dimensions of $[LT^{-1}]$, from the fluid phase to the boundary of the biofilm's boundary.

At the same time, contaminants are also being diffused into the biofilm layer as again governed by an assumed first-order process.

$$-\frac{\frac{\partial S_1^*}{\partial x_i^*}}{|\nabla S_1^*|} \cdot \left(D_p^* \frac{\partial c_p^*}{\partial x_i^*} \right) = k_{p,fb} c_p^*, \quad x^* \subset \Omega_{fB} \quad (8.2.4)$$

where $k_{p,fb}$ the unknown attachment rate of contaminants, having the dimensions of $[LT^{-1}]$, from the fluid phase to the boundary of the biofilm's boundary.

Note that the physical adsorption mechanism of the contaminants/microbes is assumed to be negligible in the model development for (8.2.3) to (8.2.4) since previous studies from Section 2.4 have justified the adsorption process contribute minimally to the biofilter's removal performance over time. As the average thickness of the idealized biofilm layer is much smaller than the average grain size, diffusion is expected to be the key transport mechanism inside the porous biofilm layer which is defined as follows.

$$\frac{\partial c_m^*}{\partial t^*} = \nabla^* \cdot (D_m^* \nabla^* c_m^*), \quad x^* \subset \Omega_B \quad (8.2.5)$$

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$$\frac{\partial c_p^*}{\partial t^*} = \nabla^* \cdot (D_p^* \nabla^* c_p^*), \quad x^* \subset \Omega_B \quad (8.2.6)$$

The local consumption rate of contaminants by the available microbes within the idealized biofilm layer then results in an unknown growth rate of the same layer over time, as supported by the rigid collector spheres. Consequently, there is again a resulting outward normal velocity (an unknown quantity) acting at the fluid-biofilm interface, as defined in (3.1.6) earlier for modelling the physical clogging condition in depth filters. Likewise, the volume conservation principle is adhered to associate the growth rate of the entire collector sphere (original collector sphere plus the idealized biofilm layer) to the local consumption rate of contaminants by the microbes present inside the porous biofilm layer around the spheres, as defined in the following form.

$$\frac{\partial d^*}{\partial t^*} = -\frac{1}{\rho_p} \frac{\partial S^*}{|\nabla S^*|} \cdot \left(D_p^* \frac{\partial c_p^*}{\partial x_i^*} \right), \quad x^* \subset \Omega_{BS} \quad (8.2.7)$$

where Ω_{BS} is the interface between the collector sphere and porous biofilm layer.

Note that the present analysis only considers the lumped growth rate of the collector spheres inside the periodic cell domain due to the growing idealized biofilm layer around the spheres, without considering any empirical mass/volume distribution of the consumed contaminants, i.e. substrate, inside the biofilm layer into biomass and extracellular polymeric substances (EPS) components over time. The boundary of each collector sphere is again regarded to be impermeable which results in the no-slip flow condition. The following additional assumptions are also undertaken to model the biological clogging condition taking place inside biofilters: (i) the characteristic lengths of macroscale biofilter (L), collector spheres (l) and microbes (l') are in the orderings of (1), (10^{-3}) and (10^{-6}) respectively; and (ii) three small length scales (ε_a), (ε_b) and (ε_c), defined as $\frac{l}{L}$, $\frac{l'}{L}$ and $\frac{l'}{l}$ respectively are adhered for the homogenization procedures. All other assumptions defined previously for modelling the physical and chemical clogging conditions in depth filters are still retained in the present analysis.

8.2.2. Homogenized representations to quantify biological clogging condition

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As mentioned earlier, the same argument from the physical clogging scenario is adhered for modelling the biological clogging condition in depth filters whereby the collector spheres, within the periodic cell domain, grow gradually over time due to the transient local consumption of contaminants by the microbes within the growing thin biofilm layer. As the biofilm layer around each collector sphere grows slowly over time, the homogenized permeability coefficient within the macroscale depth filter will reduce gradually at the same time. Hence, the same homogenized representation from (3.3.3) can be adhered for estimating the filter's rate of permeability reduction during the biological clogging stage at the ordering importance of ε . In the next two sub-sections, the focus is to provide the quantitative details which can quantify the complex reactions taking place at the following domains: (a) interphase between fluid and boundary of biofilm layer; and (b) within the porous biofilm layer.

At the fluid-biofilm interface, we introduce the following alternative multiple-scale coordinates of x and $x' = \varepsilon_a x$ to expand (8.2.1) and (8.2.2) in the following.

$$-\frac{\frac{\partial S_1}{\partial x_i}}{|\nabla S_1|} \cdot \left(\frac{\partial}{\partial x_i} + \varepsilon_a \frac{\partial}{\partial x_{i'}} \right) (c_m^{(0)} + \varepsilon_a c_m^{(1)} + \dots) = \varepsilon_a (D_{m,fb}) (c_m^{(0)} + \varepsilon_a c_m^{(1)} + \dots),$$

$$x \subset \Omega_{fB} \quad (8.2.8)$$

$$-\frac{\frac{\partial S_1}{\partial x_i}}{|\nabla S_1|} \cdot \left(\frac{\partial}{\partial x_i} + \varepsilon_a \frac{\partial}{\partial x_{i'}} \right) (c_p^{(0)} + \varepsilon_a c_p^{(1)} + \dots) = \varepsilon_a (D_{p,fb}) (c_p^{(0)} + \varepsilon_a c_p^{(1)} + \dots),$$

$$x \subset \Omega_{fB} \quad (8.2.9)$$

At the leading order, $c_{m,p}^{(0)}$ from the homogenized forms of (8.2.8) and (8.2.9) are determined to be independent of the microscale variations. At the next order of ε_a for (8.2.8) and (8.2.9), the following representations are derived:

$$\begin{aligned} \frac{\partial c_{m,p}^{(0)}}{\partial t_c} + \frac{\partial u_i^{(1)} c_{m,p}^{(0)}}{\partial x_i} + \frac{\partial u_i^{(0)} c_{m,p}^{(0)}}{\partial x_{i'}} + \frac{\partial u_i^{(0)} c_{m,p}^{(1)}}{\partial x_i} \\ = (Pe_l)^{-1} (\nabla \cdot \nabla c_{m,p}^{(1)} + \nabla \cdot \nabla' c_{m,p}^{(0)} + \nabla' \cdot \nabla c_{m,p}^{(0)}), \\ x \subset \Omega_f \quad (8.2.10) \end{aligned}$$

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where $Pe_l = \frac{Ul}{D_{m,p}^*}$, and (8.2.10) is subjected to the boundary conditions of (8.2.3) and (8.2.4) for the transport of microbes and contaminants respectively as follows:

$$-\frac{\frac{\partial S_1}{\partial x_i}}{|\nabla S_1|} \cdot \left(\frac{\partial c_{m,p}^{(1)}}{\partial x_i} + \frac{\partial c_{m,p}^{(0)}}{\partial x_i'} \right) = c_{m,p}^{(0)}, \quad x \in \Omega_{fB} \quad (8.2.11)$$

Using (8.2.11) and the periodic boundary conditions for the fluid parameters, the homogenized representation which quantifies the coupled transport-reaction mechanism of the contaminants and microbes, at the ordering of ε_a , can be expressed as follows:

$$\theta_f(x, t) \frac{\partial c_{m,p}^{(0)}}{\partial t} + \tilde{u}_i^{(0)}(x, t) \frac{\partial c_{m,p}^{(0)}}{\partial x_i'} = -Pe_l^{-1} \frac{|S(x, t)|}{|\Omega|_V} \frac{1}{\alpha_{m,p}} \frac{\partial d}{\partial t} \quad (8.2.12)$$

where $\theta_f(x, t)$ is the changing porosity within the periodic cell domain.

At the next ordering importance of $(\varepsilon_a)^2$, the below representation is derived which again links the transport mechanism to the reaction processes occurring at the interphase between the fluid and biofilm boundary.

$$\begin{aligned} \theta_f(x, t) \frac{\partial c_{m,p}^{(1)}}{\partial t} + \tilde{u}_i^{(0)}(x, t) \frac{\partial c_{m,p}^{(1)}}{\partial x_i'} + \tilde{u}_i^{(1)}(x, t) \frac{\partial c_{m,p}^{(0)}}{\partial x_i'} \\ = Pe_l^{-1} \theta_f(x, t) \frac{\partial}{\partial x_i'} \left(\frac{\partial c_{m,p}^{(0)}}{\partial x_i'} \right) - Pe_l^{-1} \frac{|S(x, t)|}{|\Omega|_V} D_{a,L} c_{m,p}^{(1)}, \end{aligned} \quad (8.2.13)$$

In both (8.2.12) and (8.2.13), the homogenized fluid flow and mass transport problems are again directly linked via the slowly changing seepage flow velocity parameter, i.e. $\tilde{u}_i^{(0)}(x, t)$, for modelling the filter's biological clogging condition. The following linear time-derivative of the averaged concentration parameter for the microbes and contaminants, i.e. $\tilde{c}_{m,p} = \theta(x, t)(c_{m,p}^{(0)} + \varepsilon_a c_{m,p}^{(1)} + \dots)$, are considered as:

$$\frac{\partial \tilde{c}_{m,p}}{\partial t} = \theta_f(x, t) \frac{\partial c_{m,p}^{(0)}}{\partial t} + \varepsilon_a \theta_f(x, t) \frac{\partial c_{m,p}^{(1)}}{\partial t} + O(\varepsilon^2) \quad (8.2.14)$$

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By using (8.2.12) and (8.2.13), (8.2.15) is obtained for (8.2.14), accurate up to $O(\varepsilon^2)$, which quantifies the averaged transport and trapping behavior of microbes and contaminants inside depth filters.

$$\begin{aligned} \frac{\partial \tilde{c}_{m,p}}{\partial t} = & -\frac{\partial(\tilde{u}_i c_{m,p})}{\partial x_{i'}} - D_{m,p} Pe_l^{-1} \frac{|S(x,t)|}{|\Omega|_V} c_{m,p} + \varepsilon_a Pe_l^{-1} \theta_f(x,t) \frac{\partial}{\partial x_{i'}} \left(\frac{\partial c_{m,p}}{\partial x_{i'}} \right) \\ & + O((\varepsilon_a)^2), \quad (8.2.15) \end{aligned}$$

Like, transient removal of the microbes and contaminants from the intake feedwater is expected to be most significant near to the filter's injection point. Hence, spatial variation to the global filter's seepage velocity occurs, which then modifies (8.2.15) into:

$$\begin{aligned} \frac{\partial \tilde{c}_{m,p}}{\partial t} = & -\tilde{u}_i(x,t) \frac{\partial c_{m,p}}{\partial x_{i'}} - c_{m,p} \frac{|S(x,t)|}{|\Omega|_V} \frac{\partial d}{\partial t} - D_{m,p} Pe_l^{-1} \frac{|S(x,t)|}{|\Omega|_V} c_{m,p} \\ & + \varepsilon_a Pe_l^{-1} \theta_f(x,t) \frac{\partial}{\partial x_{i'}} \left(\frac{\partial c_{m,p}}{\partial x_{i'}} \right) + O((\varepsilon_a)^2), \quad (8.2.16) \end{aligned}$$

where $D_{m,p} = \frac{kl}{\varepsilon_a D_{m,p}^*}$ and $Pe_l = \frac{Ul}{D_{m,p}^*}$ for modelling the reaction taking place at the fluid-biofilm interface inside depth filters.

Quasi-steady-state biological clogging condition and one-dimensional filtration flow are again assumed to simplify (8.2.16). By doing so, the exact solution to the simplified form of (8.2.16) will be identical to (3.3.9 – 3.3.11), for modelling the physical clogging condition in depth filters, which can quantify the removal of the microbes and contaminants along the media depth over sufficiently long periods. In general, the above quantitative analysis, at the present preliminary stage, demonstrates that the complex biological clogging condition taking place inside depth filters can be simplified with the same conceptual argument as that of the physical clogging condition from the previous sub-section. By doing so, the breakthrough phase of depth filters undergoing the biological clogging behavior can also be controlled by the transient reduction in its average permeability coefficient as explained earlier. Future research work emphasizes on quantifying the complex diffusion-reaction mechanism of the diffused contaminants inside the biofilm layer, resulting in the transient rise in the mass/volume

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of biomass and EPS components within the same layer based on mass balance principles.

Adopting the respective terms from (8.2.16) at the ordering importance of ε_a , the final expression, under quasi-steady-state clogging condition, is obtained as follows.

$$0 = -\tilde{u}_i(x, t) \frac{\partial c_{m,p}}{\partial x_{i'}} - c_{m,p} \frac{|S(x, t)|}{|\Omega|_V} \frac{\partial d}{\partial t} - D_{m,p} Pe_l^{-1} \frac{|S(x, t)|}{|\Omega|_V} c_{m,p}, \quad (8.2.17)$$

By again using the homogenized Darcy's Law representation ($\tilde{u}_K(x_K, t) = -\tilde{k}(x_K, t) \frac{\partial p}{\partial x_{K'}}$) in its averaged form for unidirectional flow (Chew and Law., 2019a, 2019b), (8.2.17) is further modified into:

$$0 = \tilde{k}(x_K, t) \frac{\partial p}{\partial x_{K'}} \frac{\partial c_{m,p}}{\partial x_{K'}} - \frac{|S(x_K, t)|}{|\Omega|_V} \left(\frac{\partial d}{\partial t} + D_{m,p} Pe_l^{-1} \right) c_{m,p}, \quad (8.2.18)$$

where $\tilde{k}$ is the average global permeability coefficient of the one-dimensional depth filter which varies slowly over space and time due to the biological clogging condition taking place.

Adhering to the influent's boundary condition of $c_{m,p}(0) = 1$, the exact solution to (8.2.18) can be expressed as:

$$\tilde{k}(x_K, t) = \frac{A_{m,p}(x_K, t)}{\ln(c_{m,p}) \left(\frac{\partial p}{\partial x_{K'}} \right)} x_{K'} + C_3 = - \frac{m_{m,p}(x_K, t)}{\left(\frac{\partial p}{\partial x_{K'}} \right)} x_{K'} + C_3, \quad (8.2.19)$$

whereby $m_{m,p}(x_K, t) = -\frac{A_{m,p}(x_K, t)}{\ln(c_{m,p})}$ and $A(x_K, t) = \frac{|S(x_K, t)|}{|\Omega|_V} \left(\frac{\partial d}{\partial t} + D_{m,p} Pe_l^{-1} \right)$ which is linked to the filter's physical parameters responsible for its biological clogging condition taking place. Likewise, C_3 in (8.2.19) is an unknown integration constant which varies between 0 and 1 since $\tilde{k}(x_K, t)$ is a dimensionless parameter and too varies between 0 and 1. Again, note that $\ln(c_{m,p})$ is always negative, i.e. $c_{m,p} < 1$, at the filter's effluent discharge point, and $\frac{\partial p}{\partial x_{K'}}$ is also a negative quantity along the media depth as gravitational force controls the downward seepage flow direction.

8.2.3. Pre-processing procedures for modelling biological clogging condition

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In the context of biological clogging behavior, $\tilde{k}(x_K, t)$ in (8.2.19) is modelled as a function of the same physical parameters from that of the physical clogging condition in Section 4.1, plus the known BET surface area of the media grains (A_g). Hence, there will be an additional dimensionless pi-term involved to quantify the complex biological clogging condition. By again adopting the repeating variables of ρ_p , g and L_m for the Buckingham pi-group theorem, the following pi-terms are obtained as:

$$\begin{aligned} \pi_1 = \tilde{k}(x_K, t), \quad \pi_2 = \frac{d_0^*}{L_m}, \quad \pi_3 = \frac{V_s}{(L_m)^{0.5} g^{0.5}}, \quad \pi_4 = \frac{c_0}{\rho_p}, \quad \pi_5 = \frac{t^* g^{0.5}}{(L_m)^{0.5}}, \\ \pi_6 = \frac{d_p}{L_m}, \quad \pi_7 = \frac{\nu}{(L_m)^{1.5} g^{0.5}}, \quad \pi_8 = \rho_p A_g L_m \end{aligned} \quad (8.2.20)$$

Likewise, the biological clogging problem is also linearized by taking the natural logarithm on both sides of (8.2.19) to derive:

$$\ln(\tilde{k}(x_K, t)) = \ln\left(-\frac{m_{m,p}(x_K, t)}{\left(\frac{\partial p}{\partial x_K'}\right)} x_K' + C_3\right) = D(x_K, t), \quad (8.2.21)$$

The lumped term of $D(x_K, t)$ is modelled same derived pi-terms from (8.2.20). Appropriate re-arrangement of the variables within the pi-terms from (8.2.20) is again performed to establish the respective quantitative relationship between each independent pi-term and $D(x_K, t)$ whereby each condition generally leads to higher $\ln(\tilde{k})$ values over time, i.e. gradual reduction of $\tilde{k}$, in (8.2.21).

- i. Invert $\frac{d_0^*}{L_m}$ as smaller grains tend to result in higher removal efficacy of the contaminants inside the biofilter
- ii. Higher V_s values increase the mass flux of contaminants into the biofilter which result in greater mass of contaminants to be removed inside the filter per unit time
- iii. Higher c_0 values have the tendency for higher mass/volume of contaminants to be removed inside the biofilter
- iv. Smaller ρ_p values usually result in greater number of contaminants to be removed inside the biofilter for each mass/volume of influent filtered

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- v. Invert $\frac{d_p}{L_m}$ as smaller-sized contaminants tend to result in greater number of contaminants to be removed inside the biofilter for each mass/volume of influent filtered
- vi. Invert $\frac{v}{(L_m)^{1.5} g^{0.5}}$ as lower fluid viscosity tends to result in higher removal efficacy of contaminants inside the biofilter for each mass/volume of influent filtered
- vii. Larger BET surface area for the media grains tend to result in higher removal performance by the biofilter

By adhering to the above-mentioned conditions, $D(x_K, t)$ can be quantified as follows:

$$B(x_K, t) = f\left(\frac{L_m}{d_0^*}, \frac{V_s}{(L_m)^{0.5} g^{0.5}}, \frac{t^* g^{0.5}}{(L_m)^{0.5}}, \frac{c_0}{\rho_p}, \frac{L_m}{d_p}, \frac{(L_m)^{1.5} g^{0.5}}{v}, \rho_p A_g L_m\right) \quad (8.2.22)$$

In (8.2.22), the pre-processed input layer is thus built for supervised learning algorithms in the following ways: (a) seven independent input features whereby each unique dimensionless pi-term represents an input feature; or (b) adopt the simplest monomial form for (8.2.22) in (8.2.23) whereby it represents a compacted input feature.

$$B(x_K, t) = n_3 \left(\frac{L_m}{d_0^*} \cdot \frac{V_s}{(L_m)^{0.5} g^{0.5}} \cdot \frac{t^* g^{0.5}}{(L_m)^{0.5}} \cdot \frac{c_0}{\rho_p} \cdot \frac{L_m}{d_p} \cdot \frac{(L_m)^{1.5} g^{0.5}}{v} \cdot \rho_p A_g L_m \right)^{n_4} \quad (8.2.23)$$

whereby n_3 and n_4 are unknown calibration constants with specific emphasis of n_3 being the weighted average of the compacted representation as the only input feature. Also, note that (8.2.23) can have a biased constant term during the model calibration step. To model the depth filter's biological clogging condition over time, experimental data, relating to the transient reduction in the filter's macroscale average permeability coefficient, was derived in this study as described in Chapter 6. Appropriate data augmentation procedures, as described in the following, are also adhered to again enlarge the size of the training data for the supervised machine learning step in the later stage.

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- i. Extract the available data points for $\ln(\tilde{k}(\varepsilon^{-1}, t))$ at the maximum media depth associated from a defined training period in the experimental run carried out in this study.
- ii. Perform linear regression analysis of $\ln(\tilde{k}(\varepsilon^{-1}, t))$ over time of the defined training period from step (i).
- iii. Check the respective high coefficient of determination (R^2) values; ensure that R^2 should be of minimum value of 0.90 (a defined arbitrary value in our analysis). If so, proceed to step (v).
- iv. Attempt a higher-order regression analysis or other types of machine learning models of the extracted measured data from step (i) and perform step (ii – iii) again. Note that very high ordering degrees are avoided whenever possible to prevent overfitting of the augmented dataset during model training.
- v. Adopt the derived fitting model from step (ii) to interpolate more training data points for $\ln(\tilde{k}(\varepsilon^{-1}, t))$ associated with the same training period defined from step (i) by using a finer time-step (resolution).
- vi. For the defined time-step from step (iv), augment the quantity of data points, to the computed quantity of $[(\text{total training period})/(\text{time-step})]$ associated with the total defined training period in throughput units defined from step (i).

In the later section, the augmented training instances are adopted to perform supervised learning, via the use of a shallow deep long-short-term-memory (LSTM) architecture, of the proposed model in (8.2.23) to quantify the biofilter's biological clogging condition in the conducted experimental run in this study.

8.2.4. Experimental simulation of chemical clogging conditions

At the end of the series of adsorption column experiments (from the previous subsection), all apparatus and equipment were disinfected with bleach solution and washed thoroughly with tap water before re-deployment. In the final set of depth filtration experiments, prolonged biological clogging condition was simulated by filtering nutrient-rich marine broth (BD, Marine Broth 2216) diluted solutions in the same experimental filter from Figure 6.1.1 after the above-mentioned disinfection stage. Note that a new set of GAC grains, having the same physical and chemical

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characteristics from that of the adsorption experiments, were used for filtering synthesized marine broth over a period of 90 days under creeping flow conditions. Before deployment, the GAC media was again washed profusely with de-ionized water before drying in the oven at 100°C for 24 hours. The GAC media depth was also maintained at 60cm.

The original powdered form of marine broth material (BD, Marine Broth 2216) has a concentration of 3.74% in solution. Diluted solutions of marine broth were prepared daily by dissolving 20g of the original powder in de-ionised water and then auto-claved appropriately. The auto-claved solution was then diluted with 80L of tap water in the built-in influent tank (Figure 6.1.1) and pumped continuously into the GAC column for a period of 72 days at a constant intake flow rate of 8.0ml/min to emulate the biofiltration mechanism under creeping flow conditions. Concentration of the intake feedwater of synthesized broth solutions ranged between 10 to 60mg/L to emulate the complexity of the real-world conditions. The column setup and influent tank were wrapped with black trash bags to prevent phototrophic microbial growth. All other tubing connections were wrapped with aluminium foil to prevent light penetration.

Prior to the start of a 72-days experimental run, incubation of the GAC column was initiated with 2L of concentrated autoclaved marine broth solution by dissolving two sets of 37.4g of its powdered form with 1L of deionized water. Before incubation, the prepared concentrated broth solution had an average of 2.64×10^{11} CFU/ml for the marine microbial plate count (BD Marine Agar 2216) with triplicate samplings. The incubation step lasted for a period of 3 days during which the clean GAC media effectively absorbed the broth materials. This was evident by an average plate count of 1.80×10^8 CFU/ml in the drained solution from the GAC column which significantly dropped from the original count as stated above. At specific timings, 50ml of samples were collected from the influent tank and at Location 8 in Figure 6.1.1 for dissolved organic carbon (DOC) concentration measurements. DOC measurements were carried out within a few hours in the laboratory after sample collections and vacuumed filtered through glass filter papers having 0.45µm pore sizes. Due to material constraints, marine microbial plate counts were only carried out for the influent and effluent samples on a weekly basis. The biofiltration

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Prior to sample collections, the glassware used were first soaked in an aqueous 10% (v/v) hydrochloric acid (HCl) solution for 24 hours and then rinsed with copious amounts of MQ water. The washed glassware was then wrapped with aluminium foil and heated to 450°C for 4 hours. For plastic materials, they were also soaked in an aqueous 10% (v/v) HCl solution for 24 hours and then rinsed with copious amounts of MQ water. Finally, all materials were sterilised by autoclaving them for 30 minutes at 121°C as a final precautionary step.

8.2.5. Model training and validation for predictive maintenance objective

The homogenized averaged representation of (8.2.19) is again coupled with the proposed dimensional analysis technique to model the complex biological clogging condition in depth filters under creeping flow condition. Unlike from the physical clogging scenario, a shallow-deep long-short-term-memory (LSTM) neural network architecture, similar to the network used in Figure 5.2.1 for modelling the physical clogging behavior under rapid flow condition, is now adopted to train (8.2.23) with an augmented pool of training instances derived from Section 8.2.3 previously.

The design of the proposed shallow-deep LSTM model is again based on trial and error and extensively varying the number of neurons in the different hidden layers is not performed for this study. Instead, the hyperparameters of learning rate, number of epochs and number of mini batches are varied accordingly with the model's training period, in terms of filter's throughput units (dimensionless term), to determine the most suitable combination of hyperparameters for the proposed LSTM model which can effectively analyse the biological clogging condition in depth filters over time. The rectified linear unit (ReLU) activation function is again attached to the neurons in the final dense layer as the function can effectively predict time-valued outputs at each neuron during every epoch run using positive input features from (8.2.23) in this study.

Likewise, direct simple regression analysis or least squares method is avoided for directly fitting the raw measured data for the $\ln(\tilde{k})$ parameter in (8.2.21) as the derived empirical equation does not link their calibrated coefficients to the physical parameters associated with the filter's biological clogging condition. Importantly, the novel engineering model must relate the hybrid variations of the known physical parameters

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to the biofilters' breakthrough timings under creeping flow conditions. The proposed LSTM model, having an optimized set of hyperparameters, provides the numerical freedom to fulfil the targeted objective by flexibly varying the pre-processed input layer from (8.2.23) and predict their hybrid effects on the depth filter's breakthrough timing due to the occurring biological clogging condition.

The following set of hyperparameters: (a) the learning rate (α_1) of values 0.01, 0.001 and 0.0001; (b) the sizes of mini-batches (α_2) of values of 1, 2, 4, 8, 16 and 32; and (c) the number of epochs (α_3) of values 50, 100 and 150, are varied accordingly for the grid-search test of the shallow-deep LSTM model by using the augmented experimental data from this thesis study. The number of neurons in each LSTM cell is fixed at 50, together with a constant dropout rate of 0.2. Based on the reported findings for modelling the physical and chemical clogging conditions in depth filters, an initial 30% training period is assumed to be most appropriate to effectively model the complex biological clogging behavior with an augmented pool of training instances. Again, note that 80% of the augmented dataset is used for investigating the above-listed combination of hyperparameters, while the remaining 20% is adopted to validate the model's predictive accuracy for the defined training period as part of the cross-validation step.

Table 8.2.1 (shown below) lists the respective root-mean-squared-error (RMSE) values derived from the comparison between LSTM model's predictions, using the calibrated weightages and biased term, and measured data (before data augmentation) from the entire training period (training plus cross-validation steps) for experimental run carried out in this study. The combination of $\alpha_1 = 0.001$, $\alpha_2 = 4$ and $\alpha_3 = 300$ is determined to result in the lowest possible RMSE value as shown in Table 8.2.1. The optimized set of hyperparameters ($\alpha_1 = 0.001$, $\alpha_2 = 8$ and $\alpha_3 = 100$), as determined from the grid-search study for the shallow-deep LSTM model, is then adhered to further test the model's predictive accuracy for the remaining 70% of the experimental filter's total operational period as shown in Figure 8.2.1. Reasonable agreement (average of 0.167 in RMSE value) is attained between the LSTM model's predictions with the respective measured data (before data augmentation), as derived

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from the present study, for modelling the $\ln(\tilde{k}(\varepsilon^{-1}, t))$ parameter during the combined training step.

Figure 8.2.1. Comparison between measured and predicted values from shallow-deep LSTM model for $\ln(\tilde{k}(\varepsilon^{-1}, t))$ parameter during training and testing stages for present experimental study of biological clogging condition in depth filters.

Figure 8.2.2: Measured c_p values from experimental analysis of biological clogging condition in this study.

Figure 8.2.1 shows that the transient variations in the measured effluent concentration of synthesized marine broth, which complex fluctuations are difficult to model effectively and remain an open research question. Hence, using the effluent concentration as the breakthrough criteria for operating biofilters may not a conservative choice at present as there are no suitable quantitative representations which can account for the complex effluent concentration behavior over time. At the same time, the concentration results from Figure 8.2.2 justify the systematic derivations of (8.2.21) for using the filter's global permeability coefficient to approximate the breakthrough phase during the biofiltration process as demonstrated in Figure 8.2.1.

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Likewise, the proposed shallow-deep LSTM model from Section 7.1.3 is leveraged to investigate the effects of varying the operational conditions on the biofilter's breakthrough timing (t_b) for predictive maintenance purposes. Again, t_b occurs when the biofilter's global permeability coefficient at its maximum media depth, i.e. $\ln(\tilde{k}(\varepsilon^{-1}, t))$, reaches its stagnation zone or sufficiently low value under creeping flow conditions as discussed previously. Based on the present model calibration results, t_b for the experimental biofilter approximates to 80 throughput units, i.e. after filtering 30mg/L of influents at 0.0272m/h for 1770 hours from the start of operations. Two unique classes of parameters variations are thus carried out for the biological clogging experiments carried out in this study, namely: (a) varying uncontrollable parameters in c_0 ; and (b) varying the controllable parameter in V_s , to evaluate their effects on the filter's breakthrough timing. For the former, Table 8.2.2 lists the predicted t_b values with accordance to each varied combination of c_0 and V_s for filtering both low- and high-concentration influents in biofilters.

Tables 8.2.2 also lists the amount of preparatory timings for each varied combination of the physical parameters based on a 30% initial training period for calibrating the proposed shallow-deep LSTM model as demonstrated in Section 7.1.3. The simulation results from Table 8.2.2 indicate that both c_0 and V_s can significantly affect the biofilter's breakthrough times as expected whereby combinations of high c_0 and V_s values can lead to faster breakthrough during operations. In summary, the trained shallow-deep LSTM model, with a reasonable early training period (30% at present) with real-world measured data and operational conditions, can be useful for field engineers to predict the timing for any arbitrary biofilter reach its breakthrough stage under creeping flow conditions, as based on the hybrid combinations of the physical parameters in (8.2.23). By doing so, significant amount of preparatory time can be provided to field engineers, after the initial model training phase, to efficiently manage the logistics and resources required for filter maintenance during the complex biofiltration process.

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Table 8.2.1. Effects of varying learning rate (α_1), number of epochs (α_2) and size of mini-batches (α_3) on LSTM model's predictive accuracy for entire training step (training + cross-validation) using experimental data derived from present study.

Combination	α_1 (learning rate)	α_2 (sizes of mini batches)	α_3 (number of epochs)	RMSE (training)
1	0.001	8	50	0.542
2	0.01	8	50	0.620
3	0.1	8	50	0.731
*4	0.001	8	100	0.167
5	0.01	8	100	0.592
6	0.1	8	100	0.687
7	0.001	8	150	0.302
8	0.01	8	150	0.627
9	0.1	8	150	0.731
10	0.001	16	50	1.04
11	0.01	16	50	0.512
12	0.1	16	50	0.663
13	0.001	16	100	0.597
14	0.01	16	100	0.542
15	0.1	16	100	0.689
16	0.001	16	150	0.312
17	0.01	16	150	0.583
18	0.1	16	150	0.731
19	0.001	32	50	0.385
20	0.01	32	50	0.443
21	0.1	32	50	1.03
22	0.001	32	100	0.890
23	0.01	32	100	0.452
24	0.1	32	100	0.659
25	0.001	32	150	0.633
26	0.01	32	150	0.468
27	0.1	32	150	0.723

*** lowest possible RMSE**

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Tables 8.2.2. Summary of predicted timings from shallow-deep LSTM model for present experimental biofilter setup to reach its breakthrough stage under varying c_0 and V_s values for predictive maintenance objective.

Combination	$c_0(kg/m^3)$	$V_s(m/h)$	$t_b(h)$	Preparatory time (h)
1	0.0300	0.0200	~2400	~1680
2	0.0300	0.0300	~1600	~1120
3	0.0300	0.0400	~1200	~840
4	0.0300	0.0500	~960	~670
5	0.0300	0.0600	~800	~560
6	0.0300	0.0700	~686	~480
7	0.0300	0.0800	~600	~420
8	0.0300	0.0900	~533	~373
9	0.0300	0.100	~480	~336
10	0.0300	0.200	~240	~168
11	0.100	0.0200	~720	~504
12	0.100	0.0300	~480	~336
13	0.100	0.0400	~360	~252
14	0.100	0.0500	~288	~202
15	0.100	0.0600	~240	~168
16	0.100	0.0700	~206	~144
17	0.100	0.0800	~180	~126
18	0.100	0.0900	~160	~112
19	0.100	0.100	~144	~101
20	0.100	0.200	~72	~50

8.2.6. Further model developments

At present, the proposed engineering model is missing of useful quantitative representations which can account for the production rates, by adhering to additional unknown parameters based on mass balance principles, of the biomass and EPS materials inside the thin idealized biofilm layer around the collector spheres. Upon doing so, appropriate normalization of those representations can again be performed prior to the same systematic homogenization procedures, however, by using an alternative perturbation parameter which now relates scaling size ratio between the characteristic lengths of the thin biofilm layer and macroscale media depth. The addition then enables us to propose a coupled relationship between the growth rate of the collector spheres and the production rate of biomass inside the idealized biofilm layer, which may be more representative of the real-world biological clogging complexity inside the biofilter system. At the same time, with closer investigations of the diffusion-reaction mechanism inside the biofilm layer, the resulting engineering

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models can be useful to estimate the layer's micro-porosity parameter, which remains an open research topic, by using the same volume-averaging technique to homogenize the diffusion-reaction representation associated with the biofilm development rate.

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Appendix A: Mathematical model development of DRFM

Supplementary A: Governing equations in DRFM

DRFM begins with the filtration kinetics principle in (A1) (Adin and Rebhun, 1977) which quantifies the accumulation rate of turbidity particles within a granular filter of unidirectional flow.

$$\frac{\partial \sigma}{\partial t} = [k_{rem} V_s c (F - \sigma)] - [k_{det} \sigma J] \quad (A1)$$

where c is the concentration, σ the specific deposit, v the unidirectional flow velocity within the filter, F the theoretical filter capacity, t the time, k_1 the removal coefficient, J the hydraulic gradient, and finally k_{det} the detachment coefficient.

DRFM assumes negligible particle detachment occurring during the effective filtration stage. (A1) can then be simplified to (A2) by using the mass balance relationship in (A3) which approximates the spatiotemporal variation of c along the unidirectional media depth.

$$\frac{\partial c(z, t)}{\partial z} = -\lambda_c(z, t) c(z, t) \quad (A2)$$

$$v \frac{\partial c}{\partial z} + \frac{\partial \sigma}{\partial t} = 0 \quad (A3)$$

where λ_c is the filter coefficient due to clogging which is assumed to vary with space and time, and z the depth. We note that λ_c in (A2) is the lumped product of $k_1(F - \sigma)$ for simplicity from the modified form of (A1).

Prior to the simulation run in DRFM, z is first discretized into multiple nodal points (n) which are regularly separated by a selected Δz value. At each time-step (Δt) during the simulation, DRFM first compute the clogging degree ($D_{c\%}(z, t)$) in (A4) for all nodes at the current time step following the volume conservation principle, by using the respective concentration values from the previous time-step. The computed ($D_{c\%}(z, t)$) values are assumed to affect $\varepsilon_c(z, t)$ in (A5) and $d_c(z, t)$ in (A6) at the respective nodes under clogging conditions at the current time-step. We note that $c(z, 0)$ equates to c_0 .

Appendix A: Mathematical model development of DRFM

$$D_{c\%}(z, t) = \left(\frac{(c_0 - c(z, t - \Delta t))V_s t}{\rho_p L_m(z) \varepsilon_0} \right) - (A4)$$

$$\varepsilon_c(z, t) = (\varepsilon_0 - D_{c\%}(z, t)) - (A5)$$

$$d_c(z, t) = (d_0^*(1 + D_{c\%}(z, t))) - (A6)$$

where d_c is the effective size of the collector grain under clogging conditions, ε_c the filter porosity under clogging conditions, L_m is the media depth, ε_0 the initial filter porosity, d_0^* the initial effective size of the collector media, V_s the superficial velocity, c_0 is the influent's concentration of turbidity particles, and ρ_p the bulk density of the turbidity particles.

During pre-treatment, the turbidity particles removed within the filter are typically within the reported size range of 20 to 100 μ m or larger as the downstream cartridge filters are built to remove this particle size range or smaller. Since DRFM is modified from the original Yao's model (Yao and O' Melia, 1968; Yao et al., 1971), the removal mechanisms of interception, gravitational sedimentation and diffusion are considered. In addition, we should note that the close packing density of the granular media within the filter is likely to render straining to be an important removal mechanism too. Studies have confirmed that straining is significant if the diameter ratio between the particle and media grain is greater than 0.15 (MWH, 2005). Traditionally, straining occurs when the average pore-size of the filter is smaller than the average turbidity particle. Intuitively, this indicates an inverse size relationship between the turbidity particle and collector grain. At this moment, the straining effect is not accounted for in Yao's model.

Since both interception and straining involve the contact of the turbidity particle with the surface of the collector grain, DRFM assumes both mechanisms into a singular removal mechanism in interception and is represented by (A7 – a) which considers the clogging effects of $d_c(z, t)$ from the current time step. In addition, DRFM includes the effect of gravitational sedimentation in (A7 – b) to remove the turbidity particles within the filter.

$$\eta_l(z, t) = 1.5 \left(\frac{d_p}{d_c(z, t)} \right)^2 \quad (A7 - a)$$

Appendix A: Mathematical model development of DRFM

$$\eta_G = \frac{d_p^2 g (\rho_p - \rho_w)}{18 \mu_{in} V_s} \quad (A7 - b)$$

where η_I the removal efficacy due to interception, η_G the removal efficacy due to gravitational sedimentation, ρ_w the density of fluid, μ_{in} dynamic viscosity of fluid, d_p the average diameter of the turbidity particle, and g the gravitational acceleration.

For rapid filtration, the effects of diffusion and electrostatic attraction forces can logically be neglected due to the considered particle size and hydraulic loading rate. On the other hand, we hypothesize that the inertial impaction mechanism is indirectly coupled with interception due to the close definitions of both mechanisms. Finally, DRFM assumes the sum of η_I and η_G to compute η_c at the current time step as follows.

$$\eta_c(z, t) = \eta_I(z, t) + \eta_G \quad (A8)$$

where η_c the filter's effective removal efficacy under clogging conditions.

We note that η_G remains a constant at all time-steps as the clogging effects of d_c is not included into (A7 – b). With respect to (A8), $\eta_c(z, t)$ is expected to gradually reduce with time as d_c grows during the effective filtration stage. DRFM then computes $\lambda_c(z, t)$ under clogging conditions at each node in (A9), which has been modified from the original Yao's model by considering the clogging effects of $\varepsilon_c(z, t)$, $d_c(z, t)$ and $\eta_c(z, t)$ as computed from (A5), (A6) and (A8) respectively at the current time step. The simulation run commences at the first Δt value and continues till the end of the run as defined by the user.

$$\lambda_c(z, t) = \frac{3(1 - \varepsilon_c(z, t))\eta_c(z, t)}{2d_c(z, t)} \quad (A9)$$

After computing (A9), DRFM proceeds to approximate c at all nodes at the current time-step by using the computed values from (A9) in (A10) below which assumes a first-order depth removal as modified from (A2).

$$c(z, t) = c_0(e^{-\lambda_c(z, t)z}) - (A10)$$

Appendix A: Mathematical model development of DRFM

Finally, DRFM computes the spatiotemporal variation of the dimensionless hydraulic gradient rate (α) at all nodes by using the modified Kozeny-Carmen (KC) equation (Carman, 1937; MWH, 2005) in (A11) under clogging conditions. It should be noted that the original KC equation was developed under non-clogging conditions. As clogging occurs with time, the percentage reduction in ε_0 should generally be more significant than the percentage increase in d_0^* which then leads to an overall increase in ΔH . For generality, (A11 – a) refers to the rate of total energy loss incurred within an operational filter, whereas (A11 – b) refers to the rate of energy loss due to effective clogging. We note that $\alpha(z, 0)$ represents the filter's energy loss under non-clogging conditions, i.e. at $t = 0$.

$$H(z, t) = 150 \frac{V_s v (1 - \varepsilon_c(z, t))^2}{g d_c^2(z, t) \varepsilon_c^3(z, t)} + 1.75 \frac{V_s^2 (1 - \varepsilon_c(z, t))}{g d_c(z, t) \varepsilon_c^3(z, t)} - (A11 - a)$$

$$\Delta H(z, t) = \frac{[H(z, t) - H(z, 0)] \Theta'_A}{H(z, 0)} - (A11 - b)$$

$$\Theta'_A = \frac{d_0^*}{d_p} - (A12)$$

where v is the kinematic viscosity of the fluid.

To account for the surface area effects of the trapped particles on $\Delta H(z, t)$, a proposed fixed length scale of Θ'_A (as computed in (A12)) is included into (A11). As our first assumption, (A12) is based on an empirical ratio between the respective sizes of a singular media grain of length d_0^* and a trapped turbidity particle of d_p size. To the best of our knowledge, we underline that this empirical ratio has not been introduced before in previous works to account for the particle size effect on the filter's energy loss rate during effective clogging conditions.

Appendix B: Mechanics of RNN and LSTM cells

Recurrent neural network is built in a manner which the output, from the previous time-step, from a concerned neuron is directly fed into itself as an input at the present time-step, hence emulating the short-term memory of a human brain. To avoid the long training time caused by vanishing/exploring gradients problem during the training step, we adopt the Long-Short-Term-Memory (LSTM) cell which is the most popular long-term memory cells (Géron, 2017). A typical LSTM cell adopted in our model is illustrated in Figure B1.

Figure B1. Simplified representation of LSTM cell.

For brevity, the state within each LSTM cell can be divided into two vectors, namely: (a) short-term state, $\mathbf{h}_t$; and (b) long-term state, $\mathbf{c}_t$. At any time-step, the current input vector ($\mathbf{x}_t$) and previous short-term state ($\mathbf{h}_{t-1}$) are fed into fully connected layers of neurons whereby the different layer serves a unique purpose as briefly described in the following (Géron, 2017).

- The main layer which outputs $\mathbf{g}_t$ based on $\mathbf{x}_t$ and $\mathbf{h}_{t-1}$ using the $\tanh()$ activation function as defined in (B1), and partially stores the layer's output in the long-term state.
- The other layers are gate controllers and use the logistic sigmoid activation function, as defined in (B2), to produce the outputs which range between 0 and 1. The outputs are fed into element-wise multiplication operations as shown in Figure 1. Hence, when the outputs are zero, the respective gate closes. Vice versa for outputs of unity value.

Appendix B: Mechanics of RNN and LSTM cells

- The forget gate determines which parts of the long-term state can be neglected.
- The input gate determines which parts of the outputs ($\mathbf{g}_t$) to be added to the long-term state, hence explaining the statement in (i).
- The output gate determines which segments of the long-term state should be read in and output at the current time-step, i.e. $\mathbf{h}_t$ and $\mathbf{y}_t$.

$$\tanh(x) = \frac{(e^x - e^{-x})}{(e^x + e^{-x})}, \quad (B1)$$

$$\sigma(x) = \frac{1}{(1 + e^{-x})}, \quad (B2)$$

In summary, RNN-LSTM is expected to encapsulate complex long-term transient patterns by first identifying the important inputs (functionality of input gate) to the analysed problem and then storing them in the long-term state. During the training step, the model learns to preserve the identified inputs for as long as possible (functionality of forget gate) and finally learn to extract them from the long-term state storage whenever they are needed. This unique functionality can be useful to extrapolate the timing for the rapid depth filter to attain its breakthrough stage, i.e. exceedance in its direct energy gradient metric due to effective physical clogging conditions.

Appendix C: Variations of training periods for modelling chemical clogging condition in adsorbers

Figure C1a: Comparison between measured and predicted values for c over varying throughput units from 10% training period of total phase-2 operational period from own experimental runs.

Figure C1b: Comparison between measured and predicted values for c over varying throughput units from 10% training period of total phase-2 operational period from referenced experiments of Treumann et al. (2014).

Figure C1c: Comparison between measured and predicted values for c over varying throughput units from 10% training period of total phase-2 operational period from referenced experiments of Zhao et al. (2016).

Appendix C: Variations of training periods for modelling chemical clogging condition in adsorbers

Figure C2a: Comparison between measured and predicted values for c over varying throughput units from 20% training period of total phase-2 operational period from own experimental runs.

Figure C2b: Comparison between measured and predicted values for c over varying throughput units from 20% training period of total phase-2 operational period from referenced experiments of Treumann et al. (2014).

Figure C2c: Comparison between measured and predicted values for c over varying throughput units from 20% training period of total phase-2 operational period from referenced experiments of Zhao et al. (2016).

Appendix C: Variations of training periods for modelling chemical clogging condition in adsorbers

Figure C3a: Comparison between measured and predicted values for c over varying throughput units from 30% training period of total phase-2 operational period from own experimental runs.

Figure C3b: Comparison between measured and predicted values for c over varying throughput units from 30% training period of total phase-2 operational period from referenced experiments of Treumann et al. (2014).

Figure C3c: Comparison between measured and predicted values for c over varying throughput units from 30% training period of total phase-2 operational period from referenced experiments of Zhao et al. (2016).

Appendix D: Calibration of n_2 parameter using different training periods in the different referenced experiments

Table D: Summary of pre-calibrated n_2 values from different training periods of entire phase-2 operational periods for the different referenced experiments.

Referenced experiment (10% training period)	n_2	$k_{ads}(m/s)$	$k_{des}(m/s)$
Present experiment (Run 1)	-1.60	2.24×10^{-10}	2.13×10^{-10}
Present experiment (Run 2)	-1.62	1.99×10^{-11}	1.89×10^{-11}
Present experiment (Run 3)	-1.57	1.65×10^{-11}	1.57×10^{-11}
Treumann et al., 2014 (Figure 4a)	2.71	2.75×10^{-9}	2.61×10^{-9}
Treumann et al., 2014 (Figure 4b)	2.25	1.41×10^{-9}	1.34×10^{-9}
Treumann et al., 2014 (Figure 4c)	1.46	4.15×10^{-9}	3.95×10^{-9}
Zhao et al., 2016 (Figure 4a)	1.11	9.29×10^{-16}	8.82×10^{-16}
Zhao et al., 2016 (Figure 4b)	1.30	4.59×10^{-17}	4.36×10^{-17}
Referenced experiment (20% training period)	n_2	$k_{ads}(m/s)$	$k_{des}(m/s)$
Present experiment (Run 1)	-1.59	5.04×10^{-11}	4.79×10^{-11}
Present experiment (Run 2)	-1.54	3.32×10^{-11}	3.16×10^{-11}
Present experiment (Run 3)	-1.55	1.99×10^{-11}	1.89×10^{-11}
Treumann et al., 2014 (Figure 4a)	2.78	2.10×10^{-9}	1.99×10^{-9}
Treumann et al., 2014 (Figure 4b)	2.36	8.10×10^{-10}	7.69×10^{-10}
Treumann et al., 2014 (Figure 4c)	1.49	3.18×10^{-9}	3.02×10^{-9}
Zhao et al., 2016 (Figure 4a)	1.18	1.02×10^{-15}	9.66×10^{-16}
Zhao et al., 2016 (Figure 4b)	1.47	9.43×10^{-20}	8.96×10^{-20}
Referenced experiment (30% training period)	n_2	$k_{ads}(m/s)$	$k_{des}(m/s)$
Present experiment (Run 1)	-1.57	5.73×10^{-11}	5.45×10^{-11}
Present experiment (Run 2)	-1.52	3.92×10^{-11}	3.72×10^{-11}
Present experiment (Run 3)	-1.51	2.89×10^{-11}	2.75×10^{-11}
Treumann et al., 2014 (Figure 4a)	2.91	1.31×10^{-9}	1.24×10^{-9}
Treumann et al., 2014 (Figure 4b)	2.41	6.27×10^{-10}	5.96×10^{-10}
Treumann et al., 2014 (Figure 4c)	1.55	1.91×10^{-9}	1.81×10^{-9}
Zhao et al., 2016 (Figure 4a)	1.33	9.41×10^{-16}	8.94×10^{-16}
Zhao et al., 2016 (Figure 4b)	1.48	9.43×10^{-20}	8.96×10^{-20}
Referenced experiment (50% training period)	n_2	$k_{ads}(m/s)$	$k_{des}(m/s)$
Present experiment (Run 1)	-1.44	8.86×10^{-11}	8.23×10^{-11}
Present experiment (Run 2)	-1.41	5.29×10^{-11}	5.03×10^{-11}
Present experiment (Run 3)	-1.48	4.02×10^{-11}	3.82×10^{-11}
Treumann et al., 2014 (Figure 4a)	2.92	7.38×10^{-10}	7.01×10^{-10}
Treumann et al., 2014 (Figure 4b)	3.01	5.09×10^{-10}	4.84×10^{-10}
Treumann et al., 2014 (Figure 4c)	2.75	1.18×10^{-9}	1.12×10^{-9}
Zhao et al., 2016 (Figure 4a)	1.31	8.01×10^{-16}	7.61×10^{-16}
Zhao et al., 2016 (Figure 4b)	1.45	1.04×10^{-16}	9.85×10^{-17}