

Physical Consistency of Axial-Dispersion Boundary Conditions and Tanks-in- Series Models for Multi-Compartment Wastewater Treatment Reactors

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Physical Consistency of Axial-Dispersion Boundary Conditions and Tanks-in-Series Models for Multi-Compartment Wastewater Treatment Reactors

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Abstract

Accurate hydrodynamic representation is essential for interpreting residence time distribution (RTD) data and for developing reliable reactor-scale models of multi-compartment wastewater treatment systems. However, the tanks-in-series (TIS) model and axial-dispersion (AD) formulations are often applied as standard RTD tools, with hydrodynamic parameters then inferred without explicit evaluation of whether the underlying transport and boundary assumptions are physically consistent with the reactor system. This study evaluates the physical consistency and predictive performance of the TIS model and AD formulations with different boundary conditions (BCs), using tracer data from a 6-L, eight-chamber anaerobic baffled reactor as a representative multi-compartment system. The reactor was operated at hydraulic retention times of 93-366 min and under changes in temperature, dissolved-solids concentration, suspended-solids concentration, and reactor scale. The AD formulations based on BC I, which applies inlet flux balance and a zero-gradient outlet, and BC III, which neglects inlet dispersion and assumes an infinite downstream domain, provided the most consistent representation of the experimental RTDs. They produced identical responses and achieved the lowest average NRMSE values: 14% across the HRT-based tests and 10% across most environmental and geometric conditions, compared with 30-31% for AD with open boundary conditions and 16-17% for TIS. Although TIS reproduced some hydrodynamic descriptors, its ideal-mixing structure gave less consistent RTD-shape agreement and can misrepresent transport in compartmentalised reactors. Breakthrough time was poorly predicted by all reduced-order formulations, showing that short-circuiting is controlled by local flow pathways not captured by global RTD models.

Keywords: Multi-compartment reactors; Wastewater treatment; Residence time distribution; Axial dispersion; Boundary conditions; Tanks-in-series

Article Highlights

- Boundary conditions strongly influence predicted residence times in treatment reactors.
- Two axial-dispersion formulations gave the closest agreement with tracer measurements.
- Complete-mixing assumptions can incorrectly predict the loss of retained biomass.

1 Introduction

Multi-compartment wastewater treatment reactors with plug-flow behaviour are widely used to improve contact between flow, substrates, solids, and biomass while reducing the limitations of single completely mixed systems. Their performance is strongly affected by non-ideal hydraulic behaviour, including backmixing, recirculation, stagnant zones, preferential pathways, and short-circuiting (Levenspiel 1999). These hydraulic features influence residence time, effective reactor volume, solids retention, and substrate-biomass contact, and therefore affect both treatment performance and the reliability of reactor-scale models.

In this study, an eight-chamber anaerobic baffled reactor (ABR) is used as a representative multi-compartment system with plug-flow behaviour. While ABRs have often been described as intermediate between ideal plug flow and complete mixing (Grobicki and Stuckey 1992; Li et al. 2016b), some studies indicate that this behaviour depends strongly on the number of compartments (Khalekuzzaman et al. 2018). ABRs with more than four or five compartments can approach non-ideal plug-flow behaviour (Xu et al. 2016), making the eight-chamber system used here a suitable experimental platform for evaluating reduced-order hydrodynamic formulations in multi-compartment reactors with plug-flow behaviour.

Hydrodynamic behaviour in wastewater treatment reactors can be represented at different levels of detail. Computational fluid dynamics (CFD) can resolve local velocity fields, recirculation zones, and spatial flow heterogeneity, but it usually requires high computational effort and becomes more complex when coupled with biokinetic models. Compartmental models provide an intermediate representation by dividing the reactor into hydraulically meaningful zones, although their development often depends on prior CFD analysis or detailed experimental characterisation. In contrast, residence-time-distribution (RTD)-based reduced-order models provide simpler reactor-scale descriptions of overall transport behaviour and are therefore widely used for interpreting tracer data and supporting reactor modelling (Haag et al. 2018; Jourdan et al. 2019).

Among RTD-based approaches, the tanks-in-series (TIS) and axial-dispersion (AD) models are commonly used to characterise reactor hydrodynamics and interpret non-ideal flow behaviour. The TIS model represents transport as a sequence of completely mixed tanks, whereas the AD model represents longitudinal spreading along the flow path using an axial dispersion coefficient. However, the AD model is not defined by the dispersion coefficient alone. Its predictions also depend on the boundary conditions imposed at the inlet and outlet, because these determine how advective and dispersive fluxes are treated at the reactor boundaries. Boundary-condition selection therefore affects not only the fitted RTD curve, but also the physical interpretation of the inferred hydrodynamic parameters.

Despite the wide use of TIS and AD formulations, their application in wastewater reactor studies has often been based on limited operating conditions or on a single assumed hydrodynamic formulation, without explicit assessment of whether the underlying hydraulic and boundary assumptions are physically consistent with the reactor being modelled. This is particularly important for AD models, where different inlet and outlet boundary conditions can lead to different RTD shapes, mean residence times, and interpretations of dispersion and effective reactor volume. If these assumptions are not examined, hydrodynamic parameters inferred from RTD modelling may reflect the imposed formulation as much as the reactor behaviour itself. This can limit the reliability and generalisability of reduced-order models, especially when they

are later used as hydraulic bases for biokinetic modelling (Liu et al. 2007; Sarathai et al. 2010; Chen et al. 2010; Ji et al. 2012; Cottorello-Fonsêca et al. 2026).

To address this gap, the present study provides, to the authors' knowledge, the first systematic evaluation of the physical consistency and predictive performance of TIS and multiple AD boundary-condition formulations for a multi-compartment reactor with plug-flow behaviour. The analysis uses an experimental RTD dataset from an eight-chamber ABR that was previously reported by the first author for flow-regime and scale-up analysis (Hassanvand Jamadi and Alighardashi 2017a, b). However, the boundary-condition dependence and physical consistency of the reduced-order hydrodynamic formulations were not examined as independent modelling decisions. Here, the dataset is re-analysed to determine whether commonly used formulations provide physically defensible representations of transport in this type of reactor. The study also links this hydrodynamic assessment to future biokinetic modelling by showing how hydraulic formulation choice can influence the interpretation of substrate transport, contact time, and model structure in ADM1-type frameworks.

2 Materials and Methods

2.1 Experimental Setup

The reactor considered in the modelling analysis was an eight-chamber anaerobic baffled reactor (ABR) with a total volume of 6 L. The reactor geometry, including the inlet and outlet configurations, is illustrated in Fig. 1. Tracer tests were conducted at six hydraulic retention times (HRTs): 93, 180, 248, 284, 332, and 366 min. The baseline experiments were performed using drinking water at room temperature (22 °C), without added dissolved or suspended solids. Four additional tests were evaluated at a baseline HRT of 180 min: elevated temperature (30 °C), dissolved solids (DS = 1000 mg/L), suspended solids (SS = 5000 mg/L), and reactor scale-up through an eightfold increase in volume. Further details of the experimental setup and tracer procedures are provided in the original experimental studies (Hassanvand Jamadi and Alighardashi 2017a, b).

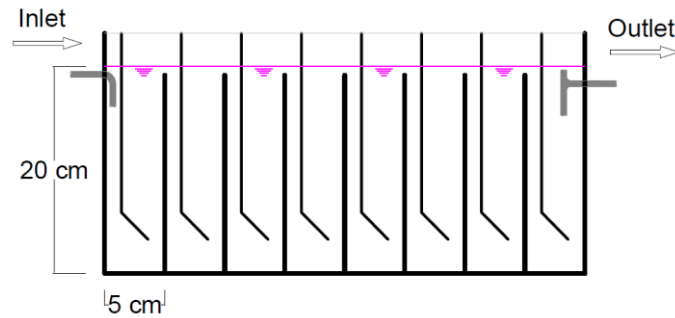


Fig. 1 Schematic representation of the experimental reactor used in this study. The total reactor volume is 6 L, with an upflow/downflow chamber volume ratio of 3. The reactor width perpendicular to the schematic plane is 7.5 cm

2.2 RTD Characterisation and Hydrodynamic Parameters

To compare experimental and model-predicted RTD curves on the same basis, the tracer responses were normalised and described using hydrodynamic parameters related to residence time, spreading, breakthrough, and peak behaviour. These parameters were used to evaluate both the agreement between measured and predicted RTDs and the physical implications of each reduced-order formulation.

The experimental RTD curve was obtained from a tracer test by plotting the outlet tracer concentration as a function of time (Hassanvand Jamadi and Alighardashi 2017b). For comparison purposes, the RTD curves were normalised using the following relationships (Tchobanoglous et al. 2003):

$$\theta = \frac{t}{\text{HRT}} \quad (1)$$

$$C_\theta = \frac{C_t}{C_0} \quad (2)$$

where t is time, HRT is theoretical retention time, and θ is the normalised time. C_t is the measured tracer concentration at time t , C_0 is the nominal concentration (tracer mass divided by reactor volume), and C_θ is the normalised concentration.

The normalised mean residence time and variance of the experimental RTD were calculated as:

$$\bar{\theta} = \int \theta C_\theta d\theta \quad (3)$$

$$\sigma_\theta^2 = \int \theta^2 C_\theta d\theta - \bar{\theta}^2 \quad (4)$$

where $\bar{\theta}$ represents the dimensionless mean residence time and σ_θ^2 is the dimensionless variance. For the discrete experimental data used in this study, the integrals were evaluated numerically using summation over the measured time intervals.

The dimensionless mean residence time is commonly used as an indicator of effective reactor volume, with deviations from unity reflecting non-ideal flow behaviour such as dead zones or internal circulation (Sarathai et al. 2010). Values of $\bar{\theta} < 1$ indicate reduced effective volume or dead zones (Tsai et al. 2012), while $\bar{\theta} > 1$ suggests extended tracer retention within the reactor.

Short-circuiting is defined as the premature passage of flow through the reactor due to non-ideal hydrodynamic conditions, such as preferential pathways or incomplete mixing (Tchobanoglous et al. 2014). In this study, the time of first tracer appearance at the outlet is used as an indicator of short-circuiting (Mullai et al. 2025).

2.3 Hydrodynamic Modelling Frameworks

2.3.1 Tanks-in-Series (TIS)

In the TIS model, the reactor is conceptualised as a series of tanks, each exhibiting complete mixing. The outlet tracer concentration is expressed as a function of dimensionless time and the number of tanks, as given by (Levenspiel 1999):

$$C_\theta = \frac{N}{(N-1)!} (N\theta)^{N-1} e^{-N\theta} \quad (5)$$

where N is the number of tanks in series, which is inversely related to the variance of the RTD curve:

$$N = \frac{1}{\sigma_\theta^2} \quad (6)$$

2.3.2 Axial Dispersion (AD)

In the AD model, radial mixing is neglected and only axial mixing is considered (Yang et al. 2008). The tracer concentration is governed by the one-dimensional advection-dispersion equation, where dispersion is characterised using the dispersion number (d) and the Péclet number (Pe), as defined below (Levenspiel 1999; Chen et al. 2010).

$$\frac{\partial C}{\partial \theta} = \left(\frac{D}{uL} \right) \frac{\partial^2 C}{\partial Z^2} - \frac{\partial C}{\partial Z} \quad (7)$$

$$d = \frac{D}{uL} \quad (8)$$

$$Pe = \frac{1}{d} = \frac{uL}{D} \quad (9)$$

where D is the axial dispersion coefficient, u is the flow velocity, L is the characteristic reactor length, and Z is the dimensionless axial coordinate (dimensionless distance from the inlet).

For systems with appreciable dispersion, the solution of the AD equation depends on the boundary conditions imposed at the reactor inlet and outlet. These boundary conditions define how advective and dispersive fluxes are treated at the reactor limits and therefore affect the resulting RTD curve and the hydrodynamic parameters inferred from it. Under the open-boundary assumption (Open BC), dispersion is treated as continuous across the reactor boundaries, and the solution is given by (Levenspiel 1999):

$$C_\theta = \frac{1}{2\sqrt{\pi\theta/Pe}} \exp \left[-\frac{(1-\theta)^2}{4\theta/Pe} \right] \quad (10a)$$

$$\sigma_\theta^2 = \frac{2}{Pe} + \frac{8}{Pe^2} \quad (10b; \text{see Online Resource 2})$$

In Eq. (10b), Pe is determined implicitly from the variance of the experimental RTD curve.

Alternative boundary-condition formulations have been proposed to represent different inlet and outlet transport assumptions. Although the theoretical influence of boundary conditions in axial-dispersion modelling has long been recognised (Ahn 1962), their physical suitability for real multi-compartment wastewater treatment reactors has rarely been evaluated systematically. In this study, four boundary-condition formulations, denoted as BC I to BC IV, were considered following Ahn (1962):

$$C_1 = C_{x \rightarrow 0^+} - \frac{D}{u} \left(\frac{\partial C}{\partial x} \right)_{x \rightarrow 0^+}, \quad \left(\frac{\partial C}{\partial x} \right)_{x \rightarrow L} = 0 \quad (11); [\text{BC I}]$$

$$C_1 = C_{x \rightarrow 0^+}, \quad \left(\frac{\partial C}{\partial x} \right)_{x \rightarrow L} = 0 \quad (12); [\text{BC II}]$$

$$C_1 = C_{x \rightarrow 0^+}, \quad \lim_{x \rightarrow \infty} C(x, t) = 0 \quad (13); [\text{BC III}]$$

$$C_1 = C_{x \rightarrow 0^+} - \frac{D}{u} \left(\frac{\partial C}{\partial x} \right)_{x \rightarrow 0^+}, \quad \lim_{x \rightarrow \infty} C(x, t) = 0 \quad (14); [\text{BC IV}]$$

where C_1 is the upstream concentration, $C_{x \rightarrow 0^+}$ is the concentration just downstream of the inlet, and x is the axial distance (dimensional) from the inlet ($x=ZL$). BC I combines a flux-balanced inlet that accounts for dispersive transport with a zero-gradient outlet. BC II neglects dispersive flux at the inlet while maintaining a zero-gradient outlet. BC III also neglects dispersive transport at the inlet and assumes an infinite downstream domain, where the concentration approaches zero at large distances.

BC IV combines inlet flux balance with the infinite-domain outlet assumption.

The analytical solutions of the AD model for non-reactive flow under each boundary condition are as follows (Ahn 1962):

BC I:

$$C_\theta = \sum_{n=1}^{\infty} \left[\frac{2\delta_n(M \sin \delta_n + \delta_n \cos \delta_n)}{(M^2 + 2M + \delta_n^2)} \exp \left[M - \left[\frac{M^2 + \delta_n^2}{2M} \right] \theta \right] \right] \quad (15a)$$

$$\sigma_\theta^2 = \frac{2}{Pe} - \frac{2}{Pe^2} (1 - e^{-Pe}) \quad (15b; \text{see Online Resource 2})$$

BC II:

$$C_\theta = \sum_{n=1}^{\infty} \left[\frac{-\alpha_n^2}{(M + M^2 + \alpha_n^2) \cos \alpha_n} \exp \left[M - \left[\frac{M^2 + \alpha_n^2}{2M} \right] \theta \right] \right] \quad (16a)$$

$$\sigma_\theta^2 \approx \frac{2}{Pe} - \frac{5}{Pe^2} \quad (16b; \text{see Online Resource 2})$$

BC III:

$$C_\theta = \left(\frac{M}{2\pi} \right)^{1/2} \theta^{-1.5} \exp \left[M - \frac{1}{2} \left[M\theta + \frac{M}{\theta} \right] \right] \quad (17a)$$

$$\sigma_\theta^2 = \frac{2}{Pe} \quad (17b; \text{see Online Resource 2})$$

BC IV:

$$C_\theta = \left(\frac{2M}{\pi} \right)^{1/2} \theta^{-\frac{1}{2}} \exp \left[M - \frac{1}{2} \left[M\theta + \frac{M}{\theta} \right] \right] - M \exp[2M] \operatorname{erfc} \left[\left(\frac{M}{2\theta} \right)^{\frac{1}{2}} + \left(\frac{M\theta}{2} \right)^{\frac{1}{2}} \right] \quad (18a)$$

$$\sigma_\theta^2 = \frac{2}{Pe} + \frac{3}{Pe^2} \quad (18b; \text{see Online Resource 2})$$

where $M = Pe/2$; δ_n and α_n are the n^{th} roots of Eqs. (19) and (20), respectively.

$$\cot \delta = \frac{1}{2} \left(\frac{\delta}{M} - \frac{M}{\delta} \right) \quad (19)$$

$$\tan \alpha = -\frac{\alpha}{M} \quad (20)$$

The series solutions in Eqs. (15a) and (16a) converged using the first six roots of Eqs. (19) and (20).

2.4 Model Performance Evaluation

To evaluate model performance, the experimentally obtained RTD curves were compared with those predicted by the TIS and AD formulations. Six model-derived RTD curves were generated for each condition: one from the TIS model, one from the AD model with open boundary conditions, and four from the AD model with alternative boundary-condition

formulations. The comparison was used to assess both predictive agreement with the experimental RTDs and the physical consistency of the hydrodynamic interpretation produced by each formulation.

Key RTD characteristics, including tracer breakthrough time, mean residence time, peak time (modal residence time), and peak concentration, were used to compare experimental and model-derived responses. Breakthrough time was used as an indicator of short-circuiting, mean residence time as an indicator of effective volume, and peak time and peak concentration as indicators of the timing and magnitude of the main tracer response.

The RMSE was used to quantify the discrepancy between the simulated and experimental RTD curves (Dan et al. 2024; Adams et al. 2025). To enable comparison across experiments with different RTD curve magnitudes, the RMSE was expressed as the normalised root mean square error (NRMSE). The NRMSE is dimensionless and is reported as a percentage for clarity, with lower values indicating improved agreement between the modelled and experimental RTD curves.

$$\text{RMSE} = \sqrt{\frac{1}{n} \sum_{i=1}^n (C_{\theta,i,\text{model}} - C_{\theta,i,\text{exp}})^2} \quad (21)$$

$$\text{NRMSE} = \frac{\text{RMSE}}{\sqrt{\frac{1}{n} \sum_{i=1}^n C_{\theta,i,\text{exp}}^2}} \quad (22)$$

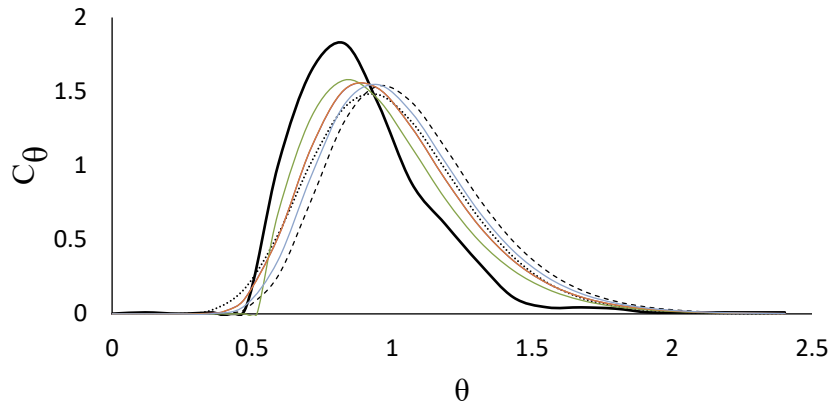
where $C_{\theta,i,\text{model}}$ and $C_{\theta,i,\text{exp}}$ represent the dimensionless tracer concentrations obtained from the model and experiment at the i th sampling point, respectively, and n is the total number of data points.

3 Results and Discussion

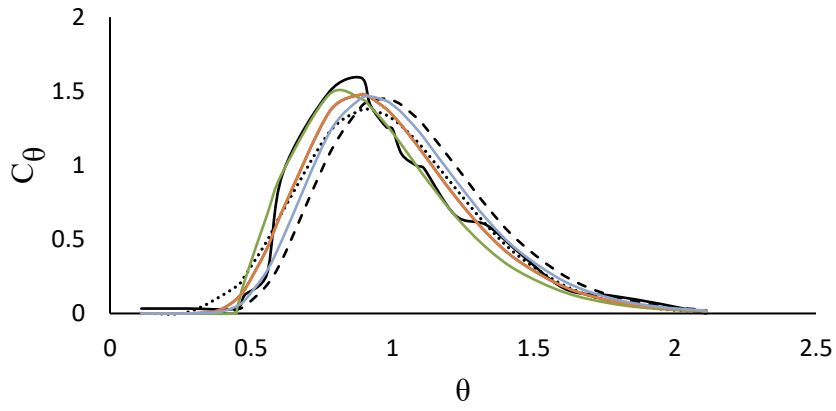
3.1 Model Performance Across Different HRTs

The experimental RTD curves were compared with those predicted by the TIS and AD formulations under different boundary-condition treatments. Representative results are shown in Fig. 2 for the lowest, intermediate, and highest HRTs, while the remaining HRT cases and detailed parameter values are provided in Online Resource 1. To ensure a consistent evaluation, a relative error threshold of 10% was adopted as the criterion for acceptable agreement in individual hydrodynamic parameters. For goodness of fit, NRMSE values below 10% were classified as excellent (He et al. 2020), while values below 15% were considered acceptable (Esrael et al. 2017). This comparison was used to examine how the reduced-order formulations respond to changes in hydraulic loading and whether their fitted responses remain physically interpretable.

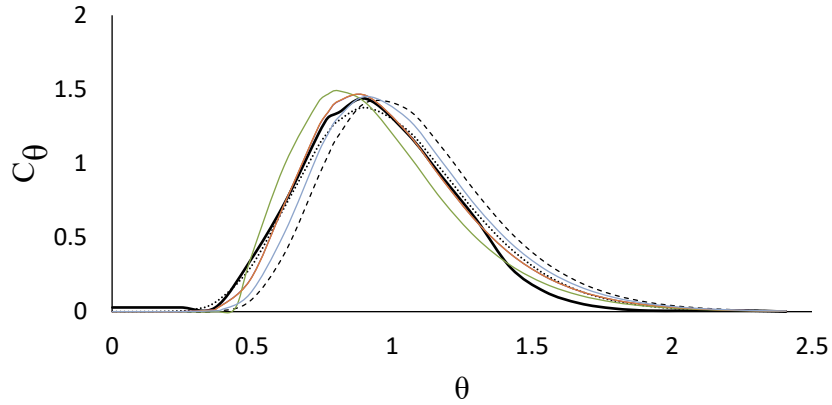
At the lowest HRT of 93 min, all formulations showed relatively large deviations from the experimental RTD, with NRMSE values ranging from 20% for BC II to 50% for Open BC. This indicates that the reduced-order formulations were less able to represent the RTD response at the lowest HRT, where local flow effects are likely to have a stronger influence on tracer transport. Model agreement improved as HRT increased. At HRT = 180 min, BC I, BC II, and BC III reached acceptable agreement, whereas Open BC remained less accurate. At an HRT of 366 min, BC I and BC III achieved excellent agreement with the experimental RTD. These two formulations produced coincident RTD curves, indicating equivalent responses over the examined range. In contrast, Open BC showed persistent deviations, suggesting that continuous dispersive exchange across the reactor boundaries can introduce systematic bias in the predicted response.



(a)



(b)



(c)

— Experimental TIS - - - Open BC — BC I — BC II — BC III — BC IV

Fig. 2 RTD curves comparing experimental data and model predictions at (a) HRT = 93 min, (b) HRT = 180 min, and (c) HRT = 366 min

3.2 Comparative Model Performance

To synthesise the HRT-based results, the modelling approaches were compared using average errors for the main hydrodynamic parameters, as summarised in Table 1. The aim of this comparison was not only to identify the lowest error

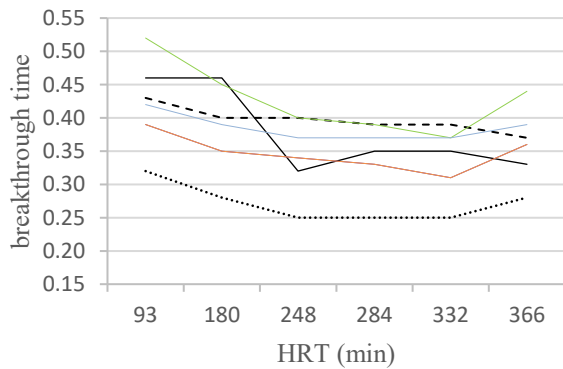
for individual RTD descriptors, but also to evaluate how consistently each formulation represented the overall RTD response and whether the resulting hydrodynamic interpretation remained physically meaningful.

Table 1 Average prediction errors of hydrodynamic parameters for evaluated formulations across different HRTs.

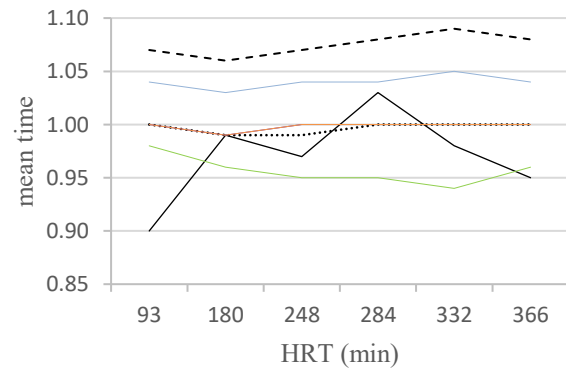
Formulation	Parameter				
	breakthrough time relative error (%)	mean time relative error (%)	peak time relative error (%)	peak concentration relative error (%)	NRMSE (%)
TIS	27	4	5	11	17
Open BC	13	11	11	8	30
BC I	12	4	5	8	14
BC II	15	5	8	9	17
BC III	12	4	5	8	14
BC IV	12	7	6	9	21
Lowest Error	BC I, III, IV	TIS, BC I, III	TIS, BC I, III	Open BC, BC I, III	BC I, III

Across the HRT range, BC I and BC III provided the most consistent overall performance, achieving the lowest average NRMSE of 14% and maintaining among the lowest average errors across the individual hydrodynamic parameters. Their identical RTD curves and hydrodynamic indices indicate that, for the range of Péclet numbers examined here, the two boundary-condition formulations were effectively equivalent in their predicted response. In contrast, Open BC produced the largest average RTD-shape deviation, with an average NRMSE of 30%, despite giving relatively low errors for some individual parameters. This finding is important because open-boundary AD formulations are sometimes adopted as simplified RTD representations, although their boundary assumptions may not be physically appropriate for compartmentalised reactors (Sarathai et al. 2010). This confirms that good agreement in an isolated descriptor does not necessarily imply a physically reliable hydrodynamic representation. TIS and BC II showed intermediate average NRMSE values of 17%, but their performance was less consistent across the HRT range. These results indicate that BC I and BC III provide the most reliable reduced-order representation for the examined multi-compartment reactor, while Open BC and TIS should be applied cautiously when RTD-derived parameters are used to infer reactor hydrodynamics.

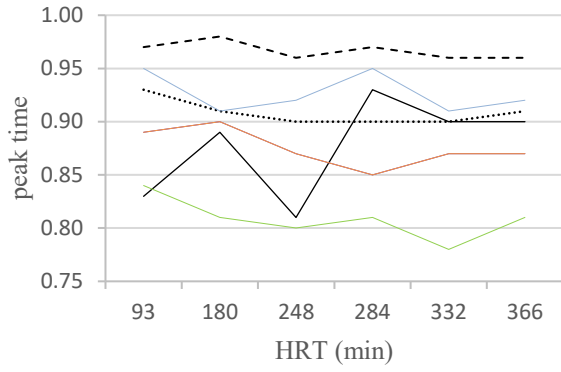
3.3 Parameter Trends with Hydraulic Loading



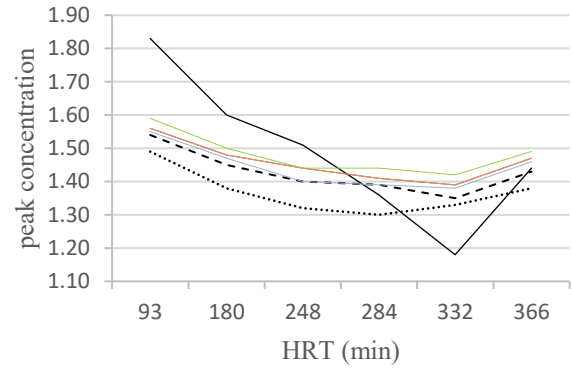
(a)



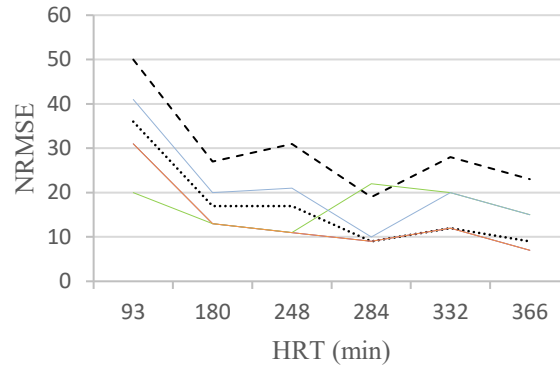
(b)



(c)



(d)



(e)

— Experimental TIS - - - Open BC — BC I — BC II — BC III — BC IV

Fig. 3 Variation of hydrodynamic parameters with HRT for the evaluated formulations

Fig. 3 compares the variation of the main hydrodynamic parameters with HRT and shows how each formulation responds to changes in hydraulic loading. The purpose of this comparison is to interpret the parameter-level behaviour behind the RTD fits reported in Sections 3.1 and 3.2.

Breakthrough time (Fig. 3a) shows no clear monotonic relationship with HRT in the experimental data, indicating that first tracer appearance, as an indicator of short-circuiting, is controlled by local flow irregularities and preferential pathways. TIS consistently predicts the earliest breakthrough because its complete-mixing structure allows rapid propagation of tracer through the tank sequence. In contrast, BC II generally predicts delayed breakthrough, reflecting its inlet boundary treatment, which neglects inlet dispersive flux and therefore limits early axial spreading. For Open BC, BC I, BC III, and BC IV, the prediction bias varies across the HRT range, confirming that breakthrough time is the least robust parameter for all reduced-order formulations.

Mean residence time (Fig. 3b) is mainly governed by the mathematical structure of each formulation. This behaviour is consistent with the moment relationships derived in Online Resource 2. TIS, BC I, and BC III all predict mean residence times close to unity, but for different mathematical reasons. In TIS, this results from representing the full reactor volume as a sequence of active, completely mixed tanks. In BC I, the flux-balanced inlet and zero-gradient outlet maintain a mass-

conservative reactor-scale response. In BC III, the mean residence time is also equal to unity, but this arises from the combination of negligible inlet dispersion and an infinite downstream domain. In contrast, Open BC and BC IV predict mean residence times greater than unity because their boundary treatments allow dispersive spreading beyond the reactor limits, producing extended apparent tracer retention. BC II gives mean residence times below unity, which is closer to several experimental values. However, this should not be interpreted as a direct physical representation of dead-zone formation. The reduction in mean residence time arises from the omission of inlet dispersive flux and should therefore be understood as a formulation-driven response.

Peak time (Fig. 3c) follows a similar formulation-dependent pattern. TIS predicts a relatively stable peak time across the HRT range and gives low average peak-time errors, but it does not capture the stronger fluctuations observed in the experimental data. Open BC and BC IV generally predict later peaks because their boundary assumptions prolong apparent tracer retention, whereas BC II predicts earlier peaks because its inlet treatment reduces effective tracer retention and shifts the concentration maximum towards shorter dimensionless times. BC I and BC III remain intermediate and produce coincident responses, showing that the two formulations behave equivalently for the examined Péclet-number range.

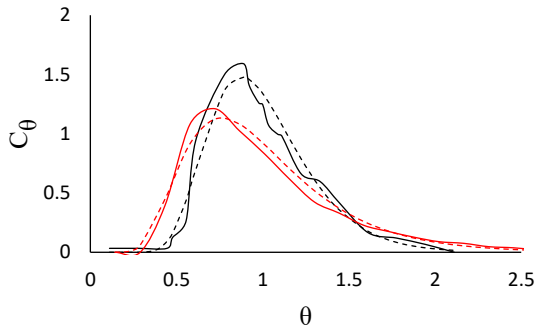
Peak concentration (Fig. 3d) also varied among the formulations. TIS generally predicted lower peak concentrations because complete mixing distributes the tracer more broadly through the tank sequence. BC II tended to produce higher peak concentrations because reduced inlet spreading preserves a more compact tracer pulse. The experimental peak concentration varied more sharply with HRT than the model predictions, suggesting that peak magnitude is sensitive to hydraulic features not fully represented by the reduced-order formulations.

The NRMSE trend (Fig. 3e) confirms that the overall RTD-shape agreement improves with increasing HRT for most formulations. BC I and BC III provide the most consistent RTD-shape agreement, while Open BC remains less accurate across the HRT range.

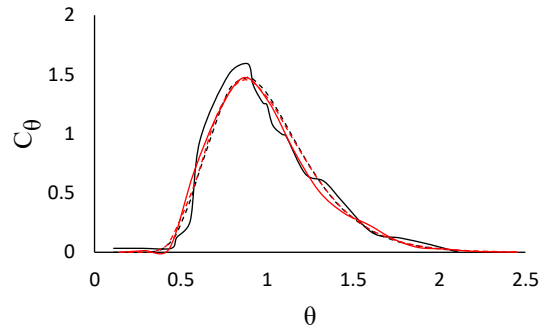
3.4 Impact of Environmental, Operational, and Geometric Conditions on Model Performance

To evaluate the sensitivity of model performance to environmental, operational, and geometric changes, four additional experiments were assessed at a baseline HRT of 180 min: elevated temperature (30 °C), dissolved solids (DS = 1000 mg/L), suspended solids (SS = 5000 mg/L), and reactor scale-up through an eightfold increase in volume under Froude similitude criteria (Hassanvand Jamadi and Alighardashi 2017a, b).

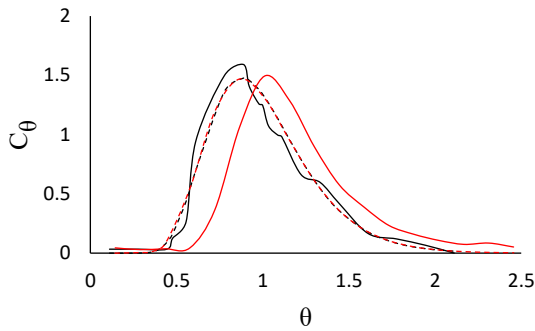
Fig. 4 compares the experimental RTDs under these conditions with the baseline response, using BC I as a representative model prediction. The complete RTD comparisons for all formulations, together with detailed hydrodynamic parameters and error indices, are provided in Online Resource 1.



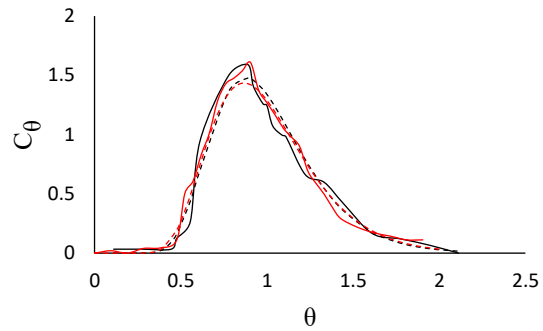
(a) Temperature (22 °C vs 30 °C)



(b) Dissolved Solids (0 vs 1000 mg/L)



(c) Suspended Solids (0 vs 5000 mg/L)



(d) Scale-up

— Baseline experimental - - - Baseline BC I — Modified experimental - - - Modified BC I

Fig. 4 Comparison of experimental RTDs and BC I under varying environmental, operational, and geometric conditions

Temperature

At an elevated temperature of 30 °C, which was associated with increased dispersion intensity and a marked reduction in the Péclet number, the experimental RTD showed delayed breakthrough relative to most formulation predictions, except Open BC. TIS, BC I, and BC III accurately predicted the mean residence time, while Open BC and BC IV overestimated apparent tracer retention. Peak time was best approximated by BC I and BC III, whereas BC II provided the closest estimate of peak concentration.

Compared with the baseline condition at 22 °C, the relative performance of the formulations remained broadly consistent. BC I and BC III provided the best overall goodness of fit at 30 °C (NRMSE = 12%), indicating that their RTD-shape agreement was maintained under increased dispersion. However, BC II showed a noticeable deterioration in RTD-shape agreement, which is consistent with its omission of inlet dispersive flux under a higher-dispersion condition.

Dissolved Solids

At a dissolved solids (DS) concentration of 1000 mg/L, the relative performance of the formulations remained broadly similar to the baseline condition. BC II provided the most accurate breakthrough-time prediction and matched the peak concentration magnitude, while TIS, BC I, and BC III gave the most accurate mean residence times. Peak time and overall RTD shape were best represented by BC I and BC III, which achieved excellent agreement with the experimental curve (NRMSE = 7%).

Compared with the baseline condition, the addition of DS did not substantially alter the hydrodynamic ranking of the formulations. However, BC I and BC III showed improved goodness of fit, while BC II no longer ranked among the best-fitting formulations. This indicates that under DS conditions, BC I and BC III provided a more consistent representation of the overall RTD response.

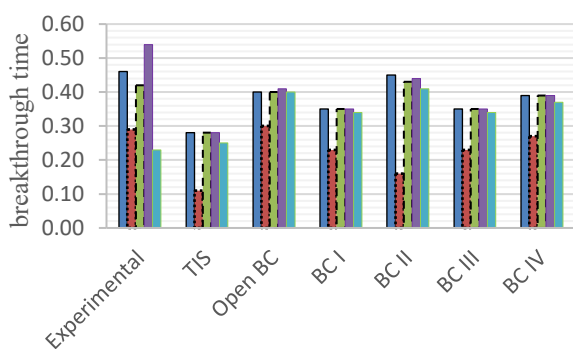
Suspended Solids

In the presence of 5000 mg/L suspended solids (SS), model performance deteriorated substantially, with NRMSE values exceeding 26% for all formulations. The experimental RTD shifted to longer residence times, with a normalised mean residence time of 1.20, indicating extended tracer retention. Unlike the previous conditions, Open BC provided the closest goodness of fit (NRMSE = 26%) and the most accurate estimates of mean residence time and peak time. This reversal occurs because the retention bias inherent in Open BC aligns with the delayed tracer response observed under high-SS conditions.

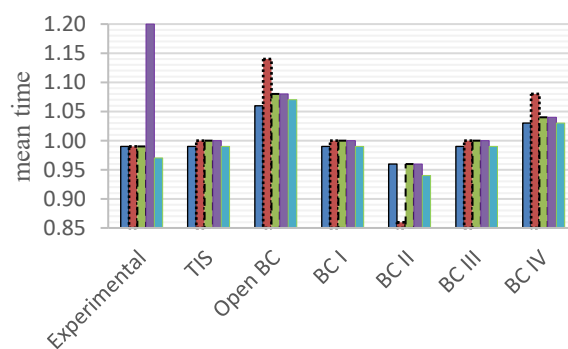
Reactor Scale-Up

Under scale-up conditions, tracer breakthrough occurred substantially earlier than in the baseline case, indicating a change in the initial hydraulic response with increasing reactor volume. TIS was the only formulation that captured this early breakthrough with acceptable accuracy, whereas all dispersion-based formulations substantially overestimated the breakthrough time.

For the remaining RTD characteristics, all formulations provided reasonable estimates of mean residence time, while TIS best predicted peak time and BC II gave the closest peak concentration. Despite their inability to capture early breakthrough, BC I and BC III again provided the best overall goodness of fit (NRMSE = 8%), indicating that these two formulations represented the overall RTD shape more reliably than the other dispersion-based formulations under scale-up conditions.



(a)



(b)

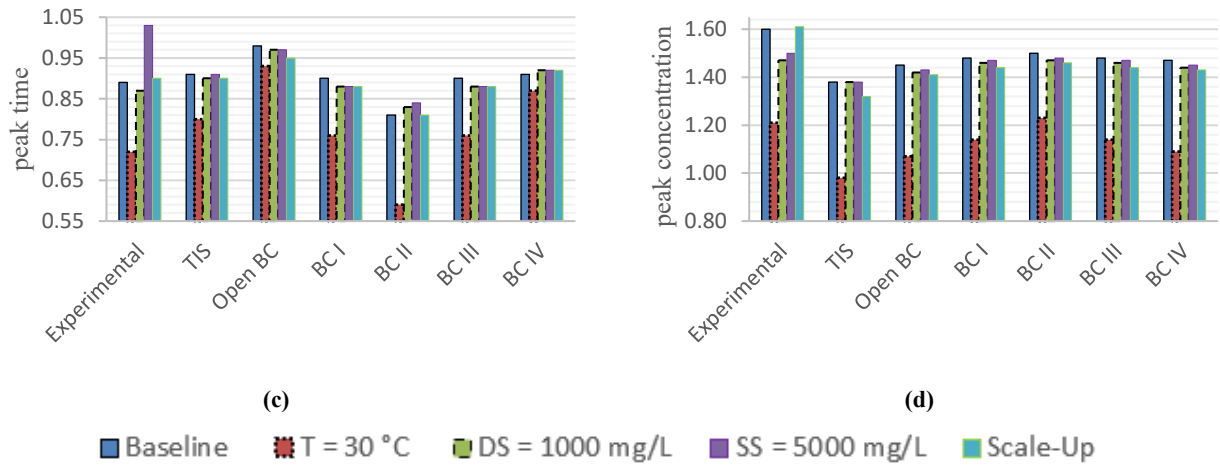


Fig. 5 Comparison of hydrodynamic parameters predicted by different formulations and experimental data under varying environmental and operational conditions

Fig. 5 compares the response of the evaluated hydrodynamic parameters under environmental, operational, and geometric perturbations. For breakthrough time (Fig. 5a), the experimental data show clear sensitivity to temperature, suspended solids, and reactor scale-up: elevated temperature and scale-up advanced tracer exit, whereas suspended solids delayed it. In contrast, the model predictions remained broadly close to their baseline values under most conditions, with the main exception being the elevated-temperature case, where increased dispersion produced a stronger shift in the predicted breakthrough response. This indicates that the reduced-order formulations had limited ability to reproduce changes that primarily affect the leading edge of the RTD curve. TIS captured the early breakthrough under scale-up more closely than the dispersion-based formulations, but this agreement should be interpreted cautiously because the experimental early exit may reflect preferential pathways or hydraulic heterogeneity rather than idealised complete mixing.

For mean residence time (Fig. 5b), the modelled responses followed the formulation-dependent behaviour discussed in Section 3.3. Under temperature, DS, and scale-up conditions, the experimental mean residence time remained close to the baseline, and most formulations showed limited change in this parameter. The main exception was the SS condition, where the experimental mean residence time increased unusually to 1.20, while model predictions remained largely unchanged. This divergence suggests that the measured RTD under high SS may not represent purely fluid-phase transport. A possible explanation is partial adsorption of Rhodamine B onto suspended particles, causing part of the tracer signal to become associated with a slower solid phase rather than the bulk liquid. In addition, particle inertia and fluid-particle interactions can modify transport and dispersion behaviour in particle-laden flows (Nanavath and Vedantam 2026). Therefore, discrepancies under high-solids conditions should be interpreted with caution, as they may reflect combined hydrodynamic and physicochemical effects rather than formulation error alone.

For peak time (Fig. 5c), the formulations responded most clearly to elevated temperature, where increased dispersion shifted the predicted concentration maximum. Under DS and scale-up conditions, both the experimental and modelled peak times remained relatively close to the baseline, indicating limited sensitivity of bulk tracer timing to these perturbations. Under SS conditions, however, the experimental peak was delayed more strongly than most model predictions, again suggesting that high solids affected tracer transport in a way not fully represented by the reduced-order fluid-phase formulations.

Peak concentration (Fig. 5d) showed a stronger experimental sensitivity than the model predictions. The experimental peak decreased under temperature, DS, and SS conditions, whereas the modelled responses changed mainly when the dispersion intensity changed substantially (30 °C). TIS generally predicted lower peak concentrations because complete mixing spreads the tracer pulse through the tank sequence, while BC II produced higher peak values because its inlet treatment preserves a more compact tracer response. Overall, Fig. 5 shows that the modelled responses are governed primarily by the fitted dispersion parameters, whereas the experimental responses also reflect condition-specific hydraulic and transport effects that are not fully captured by the reduced-order formulations.

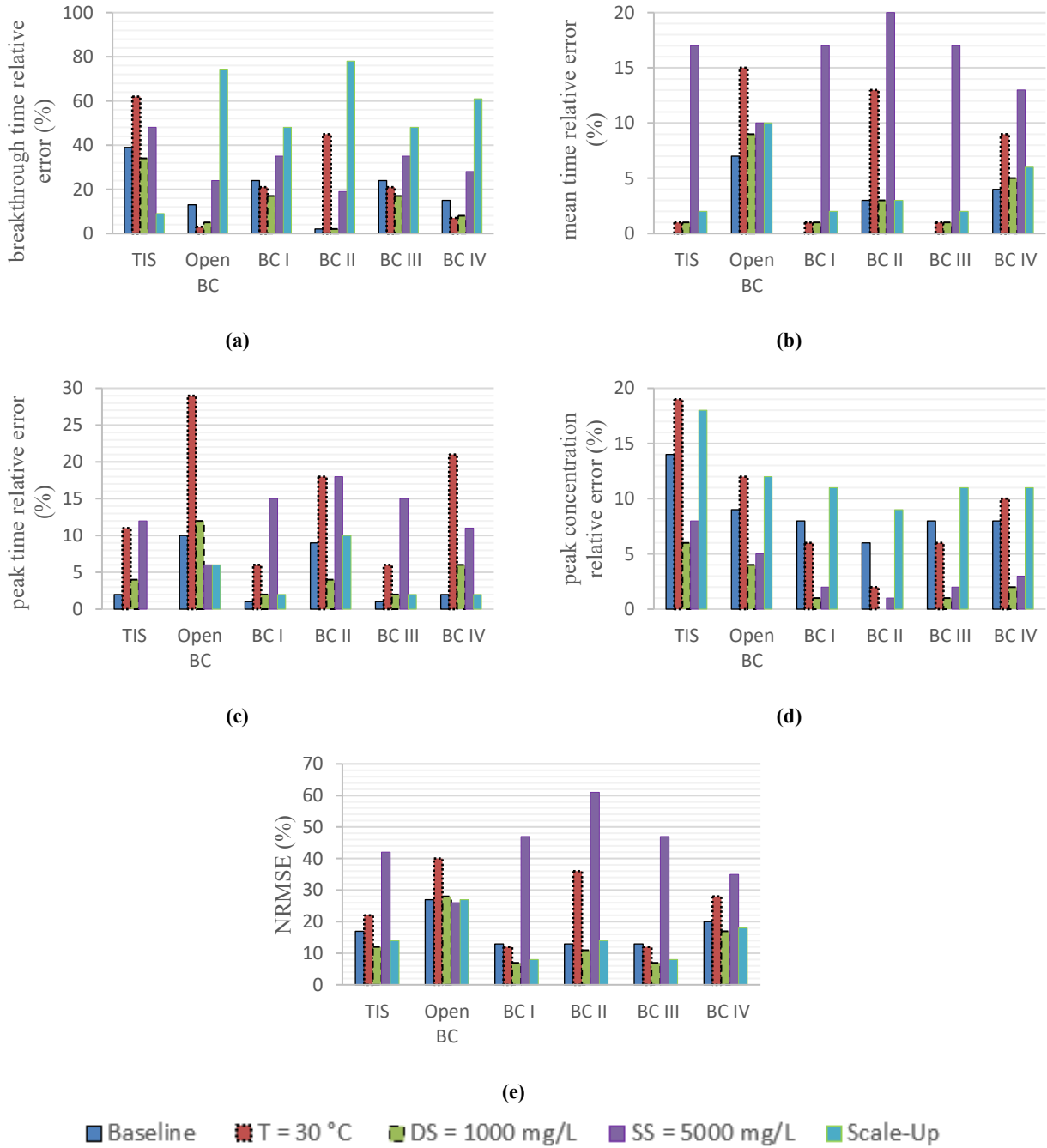


Fig. 6 Prediction errors of hydrodynamic parameters across different formulations under varying environmental and operational conditions

Fig. 6 illustrates the prediction errors of the evaluated hydrodynamic parameters under environmental, operational, and geometric conditions. Breakthrough time (Fig. 6a) remained the least reliably predicted parameter, with errors frequently exceeding the 10% threshold. This confirms that early tracer exit is strongly influenced by local hydraulic features, such as preferential pathways and short-circuiting, which are not explicitly represented in the reduced-order formulations.

Mean residence time errors (Fig. 6b) were generally low under the baseline, DS, and scale-up conditions, but increased markedly under the high-SS condition. This supports the interpretation that the SS response was affected by additional transport mechanisms beyond purely fluid-phase advection and dispersion. Peak-time errors (Fig. 6c) followed a similar pattern: most formulations performed reasonably under baseline, DS, and scale-up conditions, whereas larger deviations occurred under elevated temperature and SS conditions.

Peak-concentration errors (Fig. 6d) show that BC II provided the closest peak-magnitude predictions in several cases, while TIS generally produced larger peak-concentration deviations because its complete-mixing structure spreads the tracer pulse more strongly. Fig. 6e shows that BC I and BC III provided the most stable overall goodness of fit, maintaining acceptable to excellent NRMSE values under the baseline, temperature, DS, and scale-up conditions. In contrast, BC II deteriorated markedly under elevated temperature, while Open BC remained outside the acceptable NRMSE range under all evaluated conditions.

Table 2 summarises the average prediction errors and goodness of fit for each formulation after excluding the high-SS condition. As discussed above, this exclusion was necessary because the measured SS response may reflect solids-related transport effects in addition to fluid-phase hydrodynamics. Including this case in the averaged hydrodynamic assessment could therefore mix fluid-phase model error with additional particle-related transport effects.

Table 2 Average prediction errors of hydrodynamic parameters for evaluated formulations under varying environmental and geometric conditions, excluding the high-suspended-solids condition (baseline HRT = 180 min; scale-up condition based on the dynamically similar reactor reported previously (Hassanvand Jamadi and Alighardashi 2017a)).

Formulation	Parameter				
	breakthrough time relative error (%)	mean time relative error (%)	peak time relative error (%)	peak concentration relative error (%)	NRMSE (%)
TIS	36	1	4	14	16
Open BC	24	10	14	9	31
BC I	28	1	3	7	10
BC II	32	6	10	4	19
BC III	28	1	3	7	10
BC IV	23	6	8	8	21
Lowest Error	BC IV	TIS, BC I, III	BC I, III	BC II	BC I, III

For the remaining conditions, breakthrough time remained difficult to predict for all reduced-order formulations, with average errors exceeding 23%. In contrast, BC I and BC III provided the most reliable overall performance, giving the lowest average NRMSE (10%) and the lowest average errors for mean residence time and peak time. Their identical RTD

profiles, hydrodynamic indices, and error metrics indicate that the two formulations responded equivalently over the evaluated reactor and parameter range. The other formulations showed larger overall deviations, with Open BC and BC IV giving substantially weaker RTD-shape agreement than BC I and BC III. These trends confirm that the strong performance of BC I and BC III was not limited to the baseline condition, but extended across temperature, dissolved-solids, and scale-up conditions.

3.5 Implications for Biokinetic Modelling

Beyond hydrodynamic evaluation, the findings of this study have important implications for biokinetic modelling frameworks such as the Anaerobic Digestion Model No. 1 (ADM1). The original ADM1 formulation is based on an ideally mixed continuous stirred-tank reactor (CSTR) representation. Therefore, when ADM1 is applied to multi-compartment systems such as ABRs, the hydraulic structure is commonly extended by treating the reactor as a series of CSTRs or as a TIS-type structure.

To examine the consequence of this assumption, a diagnostic simulation was conducted in MATLAB using the experimental conditions reported by Krishna et al. (2009) for an eight-compartment ABR operated at an HRT of 10 h and an influent COD concentration of 0.5 kg COD/m³. As shown in Fig. 7, the unmodified TIS-ADM1 configuration, in which each compartment was treated as an ideal CSTR, resulted in rapid biomass washout, with solids concentration decreasing towards zero and effluent COD approaching the influent concentration. This represents modelled process failure, despite the stable treatment performance reported experimentally.

This discrepancy highlights a limitation of embedding ADM1 within a purely ideal-mixing hydraulic framework for compartmentalised reactors. The instantaneous-mixing assumption can accelerate biomass transport through the modelled reactor and remove biomass faster than realistic growth and retention mechanisms allow. This explains why empirical corrections, such as biomass retention factors, are commonly introduced in ABR modelling studies (Li et al. 2016a; Shi et al. 2019). Although such corrections can stabilise simulations, they are usually applied to the solid phase and do not fully resolve the underlying hydraulic simplification.

This analysis is intended as a diagnostic illustration rather than a full biokinetic calibration. Nevertheless, it demonstrates that hydraulic assumptions can strongly influence biokinetic predictions in multi-compartment wastewater treatment reactors. Inappropriate hydraulic representations may therefore lead to qualitatively incorrect process predictions, even when the underlying biokinetic model is well established. The formulations identified in this study as more consistent with the experimental RTD behaviour, particularly BC I and BC III, may provide a stronger basis for future coupling of RTD-based transport models with ADM1-type biokinetic frameworks.

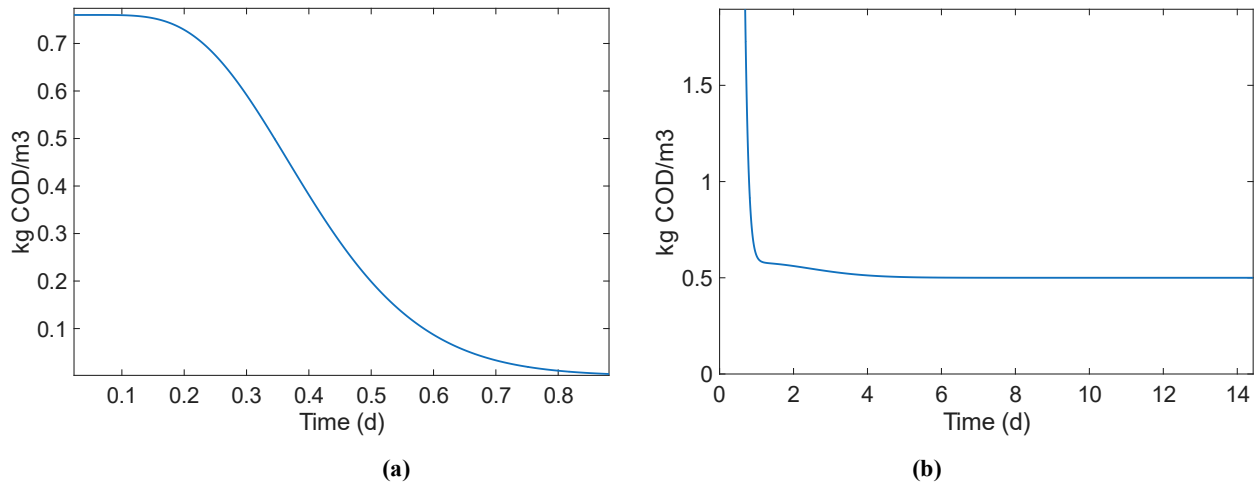


Fig. 7 Diagnostic simulation of ADM1 performance within a TIS-based hydrodynamic representation under the experimental conditions reported by Krishna et al. (2009): (a) rapid washout of methanogenic biomass (X_{ac}) in the final reactor compartment; and (b) effluent COD concentration approaching the influent loading level (0.5 kg COD/m³), indicating loss of treatment performance due to biomass washout

4 Conclusions

This study evaluated the physical consistency and predictive performance of the TIS model and several AD formulations for RTD modelling of a multi-compartment reactor with plug-flow behaviour. Across the HRT-based tests, BC I and BC III provided the most consistent representation of the experimental RTDs, producing identical responses and achieving the lowest average NRMSE of 14%, compared with 30% for Open BC. Their performance also remained strongest across the non-SS environmental and geometric conditions, where they achieved the lowest average NRMSE of 10% and the lowest average errors for mean residence time and peak time.

The results show that, within the AD model, boundary-condition selection is not a secondary numerical detail, but a controlling modelling decision that affects both RTD-shape agreement and hydrodynamic interpretation. Open BC produced the largest RTD-shape deviations, indicating that continuous dispersive exchange across reactor boundaries can introduce systematic bias in compartmentalised wastewater treatment reactors. Separately, the TIS model reproduced some hydrodynamic descriptors, but its ideal-mixing structure reduced its consistency across conditions. Breakthrough time remained difficult to predict for all reduced-order formulations, confirming that early tracer arrival, as an indicator of short-circuiting, is governed by local hydraulic features not resolved by global RTD models.

The high-SS condition produced an unusually delayed tracer response and substantially increased modelling errors for all formulations, with NRMSE values exceeding 26%. This suggests that the measured RTD may include solids-related transport effects in addition to fluid-phase hydrodynamics. This condition should therefore be interpreted cautiously when assessing fluid-phase RTD formulations.

The findings also have implications for biokinetic modelling. The diagnostic ADM1 simulation showed that using an unmodified ideal CSTR-in-series hydraulic structure can produce unrealistic biomass washout in multi-compartment reactors. Future ADM1-type models of multi-compartment wastewater treatment reactors should therefore employ

transport representations that are physically consistent with measured RTD behaviour and appropriately represent biomass transport and retention.

Supplementary Information

Online Resource 1 Additional RTD curves and detailed hydrodynamic parameters

Online Resource 2 Transfer functions and moment relationships for the evaluated RTD formulations

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Statements and Declarations

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Competing Interests

The authors have no relevant financial or non-financial interests to disclose.

Author Contributions

Mehdi Hassanvandjamadi contributed to the study conception and design, methodology, investigation, data curation, formal analysis, validation, visualisation, preparation of the original manuscript draft, and review and editing of the manuscript. Soroosh Sharifi and Bruno Fraga contributed to the study conception, methodology, supervision, and review and editing of the manuscript. All authors commented on previous versions of the manuscript and read and approved the final manuscript.

Data Availability

The experimental residence time distribution data analysed in this study were generated in earlier work by the first author and were previously reported in the publications cited in the manuscript. The derived model results and summary data supporting the findings of the present study are included in the article and its Supplementary Information.

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