Supplementary Information for:

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

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Online Resource 2

Transfer functions and moment relationships (mean time and variance) for the evaluated RTD formulations

This online resource presents the transfer functions and moment relationships used for the tanks-in-series (TIS) model and axial-dispersion formulations.

B.1 General Moment Relations

For a normalised impulse RTD, $C(\theta)$, the transfer function is the Laplace transform of the outlet response:

$$W(s) = \int_0^\infty C(\theta) e^{-s\theta}\, d\theta, \qquad W(0) = 1 \tag{B.1}$$

Differentiation of $W(s)$ gives the raw moments:

$$W'^{(0)} = -\int_0^\infty \theta\, C(\theta)\, d\theta = -\bar{\theta} \quad , \qquad W''(0) = \int_0^\infty \theta^2\, C(\theta)\, d\theta \tag{B.2}$$

Therefore,

$$\sigma_\theta^2 = \int_0^\infty \theta^2\, C(\theta)\, d\theta - \bar{\theta}^{\,2} = W''^{(0)} - [W'(0)]^2 \tag{B.3}$$

Equivalently, using the logarithm of the transfer function gives the cumulants directly:

$$\bar{\theta} = -\frac{d\ln W}{ds}\bigg|_{s=0} \quad , \qquad \sigma_\theta^2 = \frac{d^2\ln W}{ds^2}\bigg|_{s=0} \tag{B.4}$$

For the axial-dispersion formulations (BCI - IV), the following notation is used:

$$M = \frac{Pe}{2}, \qquad \beta = \left(1 + \frac{2s}{M}\right)^{1/2} \tag{B.5}$$

At $s = 0$:

$$\beta = 1 \quad , \qquad \beta_s = \frac{d\beta}{ds}\bigg|_{s=0} = \frac{1}{M} \quad , \qquad \beta_{ss} = \frac{d^2\beta}{ds^2}\bigg|_{s=0} = -\frac{1}{M^2}$$

B.2 Transfer-Function Derivation

B.2.1 Tanks-in-series model

For N equal ideal tanks in series, the dimensionless tracer balance for tank i is:

$$\frac{1}{N}\frac{dC_i}{d\theta} = C_{i-1} - C_i \tag{B.6}$$

Taking the Laplace transform and assuming zero initial tracer concentration gives:

$$\frac{s}{N} C_i(s) = C_{i-1}(s) - C_i(s) \tag{B.7}$$

Therefore,

$$\frac{C_i(s)}{C_{i-1}(s)} = \frac{1}{1+s/N} \tag{B.8}$$

For N identical tanks in series, the total transfer function is

$$W_{TIS}(s) = \left(1 + \frac{s}{N}\right)^{-N} \tag{B.9}$$

B.2.2 Axial-dispersion formulation with Open BC

The normalised open-open RTD response is written as:

$$C_{open}(\theta) = \left(\frac{M}{2\pi\theta}\right)^{1/2} \exp\left[-\frac{M(1-\theta)^2}{2\theta}\right] \tag{B.10}$$

The transfer function is obtained from:

$$W_{open}(s) = \int_0^{\infty} C_{open}(\theta) e^{-s\theta}\, d\theta$$

Expanding the exponent and applying the standard integral

$$\int_0^{\infty} \theta^{-1/2} e^{-a\theta - b/\theta}\, d\theta = \sqrt{\frac{\pi}{a}}\, e^{-2\sqrt{ab}}$$

Gives:

$$W_{open}(s) = \beta^{-1} e^{M(1-\beta)} \tag{B.11}$$

B.2.3 Axial-dispersion formulation with BC I-IV

For a non-reactive tracer, the dimensionless axial-dispersion equation is:

$$\frac{\partial C}{\partial \theta} = \frac{1}{2M}\frac{\partial^2 C}{\partial Z^2} - \frac{\partial C}{\partial Z} \tag{B.12}$$

Taking the Laplace transform with respect to θ, assuming zero initial tracer concentration, gives:

$$\frac{d^2 C}{dZ^2} - 2M\frac{dC}{dZ} - 2MsC = 0$$

The solution is obtained by assuming $C(Z, s) = e^{rZ}$, which gives the characteristic equation:

$$r^2 - 2Mr - 2Ms = 0$$

The two roots are:

$$r_1 = M(1+\beta) \quad , \quad r_2 = M(1-\beta)$$

and therefore, the general Laplace-domain concentration profile is

$$C(Z, s) = A_1 e^{M(1+\beta)Z} + A_2 e^{M(1-\beta)Z} \tag{B.13}$$

The axial derivative is:

$$\frac{dC}{dZ} = M(1+\beta)A_1 e^{M(1+\beta)Z} + M(1-\beta)A_2 e^{M(1-\beta)Z} \tag{B.14}$$

Different boundary conditions in Laplace domain are defined as follows:

flux-conserving inlet: $$C_{in}(s) = C(0, s) - \frac{1}{2M}\frac{dC}{dZ}\bigg|_{Z=0} \tag{B.15}$$

concentration-continuity inlet: $$C_{in}(s) = C(0, s) \tag{B.16}$$

zero-gradient outlet: $$\frac{dC}{dZ}\bigg|_{Z=1} = 0 \tag{B.17}$$

infinite outlet: $$C(Z, s) \to 0 \quad \text{as} \quad Z \to \infty \tag{B.18}$$

The transfer function is defined as:

$$W(s) = \frac{C_{out}(s)}{C_{in}(s)} = \frac{C(1, s)}{C_{in}(s)} \tag{B.19}$$

B.2.3.1 BC I: inlet dispersion and zero-gradient outlet

For the zero-gradient outlet condition:

$$\left.\frac{dC}{dZ}\right|_{Z=1} = 0$$

which gives:

$$A_1 = -\frac{1-\beta}{1+\beta} e^{-2M\beta} A_2$$

Substituting this relationship into $C(1,s)$ and into the flux-conserving inlet condition gives:

$$W_I(s) = \frac{4\beta e^M}{(1+\beta)^2 e^{M\beta} - (1-\beta)^2 e^{-M\beta}} \tag{B.20}$$

B.2.3.2 BC II: no inlet dispersive flux and zero-gradient outlet

The zero-gradient outlet condition is the same as in BC I, so:

$$A_1 = -\frac{1-\beta}{1+\beta} e^{-2M\beta} A_2$$

However, the inlet condition is now $C_{in}(\mathrm{s}) = C(0,s)$. Substitution gives:

$$W_{II}(s) = \frac{2\beta e^M}{(1+\beta) e^{M\beta} - (1-\beta) e^{-M\beta}} \tag{B.21}$$

B.2.3.3 BC III: no inlet dispersion and infinite downstream domain

For s > 0, β > 1. Therefore, the exponential term with the positive exponent ($e^{M(1+\beta)Z}$) grows without bound as Z tends to infinity, whereas the exponential term with the negative exponent ($e^{M(1-\beta)Z}$) decays to zero. The infinite-outlet condition requires:

$$A_1 = 0$$

Therefore,

$$C(Z,s) = A_2 e^{M(1-\beta)Z}$$

Using $C_{in}(\mathrm{s}) = C(0,s) = A_2$ and $C_{out} = C(1,s)$ gives:

$$W_{III}(s) = e^{M(1-\beta)} \tag{B.22}$$

B.2.3.4 BC IV: inlet flux balance and infinite downstream domain

The infinite-outlet condition again gives $A_1 = 0$, so:

$$C(Z,s) = A_2 e^{M(1-\beta)Z}$$

The flux-conserving inlet condition gives:

$$C_{in}(\mathrm{s}) = C(0,s) - \frac{1}{2M}\left.\frac{dC}{dZ}\right|_{Z=0} = \frac{1+\beta}{2} A_2$$

Since $C_{out} = A_2 e^{M(1-\beta)}$, the transfer function is:

$$W_{IV}(s) = \frac{2e^{M(1-\beta)}}{1+\beta} \tag{B.23}$$

B.3 Summary of Transfer Functions

Table B.1 Summary of transfer functions for different formulations

Formulation	Transfer Function
TIS	$W_{TIS}(s) = \left(1 + \frac{s}{N}\right)^{-N}$
Open BC	$W_{open}(s) = \beta^{-1} e^{M(1-\beta)}$
BC I	$W_I(s) = \frac{4\beta e^M}{(1+\beta)^2 e^{M\beta} - (1-\beta)^2 e^{-M\beta}}$
BC II	$W_{II}(s) = \frac{2\beta e^M}{(1+\beta) e^{M\beta} - (1-\beta) e^{-M\beta}}$
BC III	$W_{III}(s) = e^{M(1-\beta)}$
BC IV	$W_{IV}(s) = \frac{2e^{M(1-\beta)}}{1+\beta}$

where N is the number of tanks in the TIS model, $\beta = (1 + 2s/M)^{1/2}$, $M = Pe/2$.

B.4 Moment Derivation from The Transfer Functions

The mean and variance are obtained using:

$$\bar{\theta} = -\left.\frac{d\ln W}{ds}\right|_{s=0} \quad , \quad \sigma_\theta^2 = \left.\frac{d^2 \ln W}{ds^2}\right|_{s=0}$$

B.4.1 Tanks-in-series model

For the TIS model,

$$\ln W_{TIS} = -N \ln\left(1 + \frac{s}{N}\right)$$

Thus,

$$\frac{d\ln W_{TIS}}{ds} = -\left(1 + \frac{s}{N}\right)^{-1}$$

and

$$\frac{d^2 \ln W_{TIS}}{ds^2} = \frac{1}{N}\left(1 + \frac{s}{N}\right)^{-2}$$

At $s = 0$:

$$\bar{\theta}_{TIS} = 1 \tag{B.24}$$

$$\sigma_{\theta,TIS}^2 = \frac{1}{N} \tag{B.25}$$

B.4.2 Open-BC axial-dispersion model

For the Open-BC model:

$$\ln W_{open} = -\ln\beta + M(1-\beta)$$

Therefore,

$$\frac{d\ln W_{open}}{ds} = -\frac{\beta_s}{\beta} - M\beta_s$$

At $s = 0$:

$$\left.\frac{d\ln W_{open}}{ds}\right|_{s=0} = -\frac{1}{M} - 1$$

Thus,

$$\bar{\theta}_{open} = 1 + \frac{1}{M} = 1 + \frac{2}{Pe} \tag{B.26}$$

The second derivative gives:

$$\sigma^2_{\theta,open} = \frac{1}{M} + \frac{2}{M^2} = \frac{2}{Pe} + \frac{8}{Pe^2} \tag{B.27}$$

B.4.3 BC I

For BC I:

$$\ln W_I = \ln(4\beta) + M - \ln D_I$$

where:

$$D_I = (1+\beta)^2 e^{M\beta} - (1-\beta)^2 e^{-M\beta}$$

At $\beta = 1$:

$$D_I = 4e^M \qquad , \qquad \left.\frac{d\ln D_I}{d\beta}\right|_{\beta=1} = M + 1$$

and

$$\left.\frac{d^2\ln D_I}{d\beta^2}\right|_{\beta=1} = -\frac{1}{2}(1 + e^{-2M})$$

Using the chain rule gives:

$$\bar{\theta}_I = 1 \tag{B.28}$$

and

$$\sigma^2_{\theta,I} = \frac{1}{M} - \frac{1}{2M^2}(1 - e^{-2M})$$

Equivalently:

$$\sigma_{\theta,I}^2 = \frac{2}{Pe} - \frac{2}{Pe^2}(1 - e^{-Pe}) \tag{B.29}$$

B.4.4 BC II

For BC II:

$$\ln W_{II} = \ln(2\beta) + M - \ln D_{II}$$

where:

$$D_{II} = (1+\beta)e^{M\beta} - (1-\beta)e^{-M\beta}$$

At $\beta = 1$:

$$D_{II} = 2e^{M}$$

$$\left.\frac{d\ln D_{II}}{d\beta}\right|_{\beta=1} = M + \frac{1}{2} + \frac{1}{2}e^{-2M}$$

and

$$\left.\frac{d^2\ln D_{II}}{d\beta^2}\right|_{\beta=1} = -\frac{1}{4} - \left(2M + \frac{1}{2}\right)e^{-2M} - \frac{1}{4}e^{-4M}$$

Using the chain rule gives:

$$\bar{\theta}_{II} = 1 - \frac{1}{2M}(1 - e^{-2M})$$

or

$$\bar{\theta}_{II} = 1 - \frac{1}{Pe}(1 - e^{-Pe}) \tag{B.30}$$

The variance is:

$$\sigma_{\theta,II}^2 = \frac{1}{M} - \frac{5}{4M^2} + \frac{2M+1}{M^2}e^{-2M} + \frac{1}{4M^2}e^{-4M}$$

Equivalently:

$$\sigma_{\theta,II}^2 = \frac{2}{Pe} - \frac{5}{Pe^2} + \frac{4(Pe+1)}{Pe^2}e^{-Pe} + \frac{1}{Pe^2}e^{-2Pe} \tag{B.31}$$

At high Pe, the exponential terms become negligible, giving:

$$\sigma_{\theta,II}^2 \approx \frac{2}{Pe} - \frac{5}{Pe^2} \tag{B.32}$$

B.4.5 BC III

For BC III:

$$\ln W_{III} = M(1-\beta)$$

Therefore,

$$\frac{d\ln W_{III}}{ds} = -M\beta_s$$

and

$$\frac{d^2\ln W_{III}}{ds^2} = -M\beta_{ss}$$

At $s = 0$:

$$\bar{\theta}_{III} = 1 \tag{B.33}$$

$$\sigma_{\theta,III}^2 = \frac{1}{M} = \frac{2}{Pe} \tag{B.34}$$

B.4.6 BC IV

For BC IV:

$$\ln W_{IV} = \ln 2 + M(1-\beta) - \ln(1+\beta)$$

Therefore,

$$\frac{d\ln W_{IV}}{ds} = -M\beta_s - \frac{\beta_s}{1+\beta}$$

At $s = 0$:

$$\bar{\theta}_{IV} = 1 + \frac{1}{2M} = 1 + \frac{1}{Pe} \tag{B.35}$$

The second derivative gives:

$$\sigma_{\theta,IV}^2 = \frac{1}{M} + \frac{3}{4M^2} = \frac{2}{Pe} + \frac{3}{Pe^2} \tag{B.36}$$

B.5 Summary of Moment Relationships

Table B.2 Summary of mean time and variance for different formulations

Formulation	Dimensionless Mean Time	Dimensionless Variance
TIS	1	$\frac{1}{N}$
Open BC	$1+\frac{2}{Pe}$	$\frac{2}{Pe}+\frac{8}{Pe^2}$
BC I	1	$\frac{2}{Pe}-\frac{2}{Pe^2}(1-e^{-Pe})$
BC II	$1-\frac{1}{Pe}(1-e^{-Pe})$	$\frac{2}{Pe}-\frac{5}{Pe^2}+\frac{4(Pe+1)}{Pe^2}e^{-Pe}+\frac{1}{Pe^2}e^{-2Pe}$
BC III	1	$\frac{2}{Pe}$
BC IV	$1+\frac{1}{Pe}$	$\frac{2}{Pe}+\frac{3}{Pe^2}$