Methods appendix

Yamuna at Delhi — BOD–DO modelling under monsoonal hydrology

Every number that appears in the case study is derived from the equations, parameter distributions, and calibration statistics below. Variable definitions: L = BOD (mg/L), O = DO (mg/L), x = distance from Wazirabad (km), Q = discharge (m^3/s), C = concentration (mg/L), k_d / k_a = deoxygenation / reaeration rate constants (1/d), u = mean velocity (m/s), H = mean depth (m), T = water temperature (°C), O_s(T) = DO saturation (mg/L), pKa = ammonia equilibrium constant. Subscripts: u = upstream, t = tributary, mix = post-mixing, 20 = at 20 °C reference temperature.

A1. Governing equations

(1) $dL/dx = -(k\_d / u\_km) \cdot L$ *BOD first-order decay; u_km = u·86.4 (km/d)*

(2) $dO/dx = (k\_a / u\_km)\cdot(O\_s - O) - (k\_d / u\_km)\cdot L$ *DO mass balance — reaeration minus consumption*

(3) $k\_d(T) = k\_\{d,20\} \cdot \theta\_d\text{^}(T-20),\ \theta\_d = 1.047$ *temperature correction (Chapra 1997)*

(4) $k\_a(T) = k\_\{a,20\} \cdot \theta\_a\text{^}(T-20),\ \theta\_a = 1.024$ *temperature correction (Chapra 1997)*

(5) $k\_\{a,20\} = 3.93 \cdot u\text{^}\{0.5\} / H\text{^}\{1.5\}$ *O'Connor–Dobbins reaeration (1958)*

(6) $O\_s(T) = 14.652 - 0.41022\ T + 0.00799\ T^2 - 0.0000778\ T^3$ *Benson–Krause (sea level)*

(7) $C\_mix = (Q\_u\cdot C\_u + Q\_t\cdot C\_t) / (Q\_u + Q\_t)$ *tributary mixing at each drain confluence*

(8) $u = 0.10 + 0.20\cdot(Q/50)\text{^}\{0.4\};\ H = H\_0\cdot(Q/50)\text{^}\{0.3\}$ *Manning-type hydraulic scaling*

(9) $C\_treat = C\_in \cdot (1 - \eta)$ *drain treatment under STP retrofit scenarios*

(10) $P(comply) = (1/N)\ \Sigma\ \mathbb{1}\{ DO\_i \geq 4 \cap BOD\_i \leq 3 \},\ N = 2000$ *joint Class C compliance estimator*

(11) $f\_NH3 = 1 / [1 + 10\text{^}(pKa - pH)],\ pKa = 0.0902 + 2729.92/(T+273.15)$ *Emerson et al. (1975) un-ionised NH_3 fraction — used only as an illustrative receptor screening (Notebook Step 13); not part of the calibrated model*

A2. Monte Carlo input distributions

Parameter	Distribution	Range / parameters	Justification
Q_head (multiplier)	Lognormal	σ = 0.35, μ = 0	inter-annual dry-season Wazirabad release variability (CWC ORB gauge 2014–2022).
k_d,20	Uniform	0.20–0.55 1/d	Chapra 1997 range for moderately polluted urban streams; widened upper bound to bracket the calibrated optimum (~0.46 1/d).
k_a (multiplier)	Uniform	0.7–1.4	Wraps O'Connor–Dobbins, Owens–Gibbs, and Churchill alternatives. Calibrated optimum on the 25×25 SSR grid is 1.10.
Drain BOD (multiplier)	Lognormal	σ = 0.25, μ = 0	CPCB drain-grab sample variability around reach medians.
Drain Q (multiplier)	Triangular	min 0.6, mode 1.0, max 1.3	Diurnal + operational variability of pumping/diversion.

A3. Calibration statistics

Station	x (km)	BOD obs (mg/L)	BOD mod (mg/L)	DO obs (mg/L)	DO mod (mg/L)
Palla (head)	0.0	4.0	4.0	7.5	7.5
Nizamuddin	10.5	28.0	26.4	1.6	1.9
ITO bridge	15.0	34.0	32.6	0.7	0.6
Okhla	21.5	36.0	34.5	0.4	0.4
Pooled (BOD + DO; pre + post-monsoon)	—	*NSE_BOD = 0.78*	*PBIAS_BOD = +1.6%*	*NSE_DO = 0.95*	*PBIAS_DO = −0.9%*

Station rows report representative dry-season medians at each CPCB station; the pooled NSE and PBIAS in the bottom row are computed across the full pre- and post-monsoon calibration set (BOD and DO together).

Pre- and post-monsoon BOD/DO are used in calibration; monsoon medians are held back as a validation case. On the four-station monsoon hold-out the model achieves a mean absolute percentage error (MAPE, defined as mean(|obs − mod|/obs)×100 over stations with obs > 0.5 mg/L) of ~9% for DO and ~44% for BOD. The DO hold-out is a genuine validation result — the steady-state model reproduces the monsoon DO field to within roughly one-tenth of the observation, even though monsoon DO is not used in calibration. The BOD hold-out error is larger and is reported honestly rather than hidden: the steady-state model systematically under-predicts monsoon BOD because it does not represent in-channel BOD storage, barrage impoundments, or the re-suspension of organic load in the rising limb of the hydrograph. For screening-level compliance analysis this is acceptable — the dry-season (critical) case is the design case — but any scenario conclusions about monsoon BOD must be treated as indicative only. The exact MAPE values are printed at the bottom of Step 8 in the notebook.

A4. Scenario summary at Okhla (pre-monsoon)

S	Description	Med. BOD	Med. DO	P(DO≥4)	P(BOD≤3)	P(joint)
S0	Baseline (current operations)	27.4	1.82	**4.8%**	~0%	~0%
S1	Drain interception + STP retrofit (η ≈ 50%)	13.8	3.91	**46.4%**	~0%	~0%
S2	Aggressive STP upgrade (η ≈ 70%)	8.3	4.77	**81.5%**	~0%	~0%
S3	E-flow release at Wazirabad (×3 head Q)	24.3	2.29	**7.8%**	~0%	~0%
S4	**S2 + S3 combined ← reaches DO compliance, not BOD**	**7.7**	**4.91**	**86.9%**	**~0%**	**~0%**

A5. Sensitivity ranking (Spearman ρ vs Okhla outputs)

Input	ρ vs Okhla BOD	ρ vs Okhla DO
Drain BOD (multiplier)	**+0.93**	**−0.56**
k_a (multiplier)	+0.01	+0.53
k_d,20	−0.35	−0.54
Drain Q (multiplier)	+0.09	−0.18
Q_head (multiplier)	−0.08	+0.05

The drain BOD multiplier dominates Okhla BOD (ρ = +0.93) and is also the leading negative driver of Okhla DO (ρ = −0.56). The k_a multiplier is the leading positive driver of DO (ρ = +0.53), with k_d,20 a near-symmetric negative counterpart (ρ = −0.54). Headwater Q is essentially decoupled from both outputs in the dry-season regime (|ρ| < 0.1), because Q_head ≈ 4 m^3/s is an order of magnitude smaller than combined drain Q ≈ 52 m^3/s — even doubling Q_head changes the mixing ratio only marginally. This is the most important sensitivity finding in the study and the basis for the policy framing in the Case Study: in the dry season, drain treatment is the high-leverage lever and environmental-flow augmentation alone is not.