1 Introduction

This repository contains the MATLAB code and data used to simulate the longitudinal transport of Dissolved Inorganic Carbon (DIC) and CO_2 evasion along a stream reach, and to reproduce the results shown in Figures 6, 7 and 8 of the manuscript.

2 Repository contents

File	Description
`Data.m`, `DataFIG6.m`, `DataFIG7.m`, `DataFIG8.m`	Contains the input structure `I` (hydraulic, morphological, chemical and physical parameters), generates the random step configuration (Poisson process) for a given `fraction_steps`, and computes hydraulic geometry (depth, velocity, cross-sectional area). Called once per simulation.
`CalculateDICfromCO2TA.m`	Computes pH, CO_2, HCO_3^-, CO_3^{2-} and DIC from Alkalinity and pCO_2, using freshwater dissociation constants (Millero, 1979). Used to set upstream/lateral boundary conditions. Requires the Optimization Toolbox (`fsolve`).
`CalculateCO2pHfromDICTA.m`	Inverse calculation: given DIC and TA (and temperature), returns CO_2, pH, HCO_3^-, CO_3^{2-} and pCO_2, solved iteratively via Newton's method. Used at every spatial node during the simulation.
`CO2_evasionfluxes.m`	Computes the energy dissipation rate, the gas transfer velocity k_{600} (Ulseth et al., 2019), the Schmidt-number-corrected k_{CO_2}, and the resulting areal CO_2 evasion flux F_{CO_2}.
`steady_state.m`	Core solver. Integrates DIC and ALK along the reach with an upwind finite-difference scheme, applies the additional CO_2 evasion "jump" at each step location, and returns the output structure `O` (DIC, ALK, pH, CO_2, HCO_3^-, CO_3^{2-}, F_{CO_2}, step evasion, energy dissipation, k_{600} along the reach).
`DIC_model.m`	Main driver script. Runs a Monte Carlo simulations across a range of `fraction_steps` (share of total elevation drop assigned to steps) and produces: (i) evaded CO_2 mass vs. SR fraction (percentile bands over stochastic realizations), and (ii) a DIC/CO_2 mass-balance check and bar-chart decomposition of fluxes (upstream/downstream/lateral, NEP, segment evasion, step evasion, carbonate buffering).
`Figure_6.m`	Reproduces Figure 6: relative change in total evaded CO_2 mass between the step-dominated and segment configurations, as a function of discharge Q, for three bed slopes.

`Figure_7.m`	Reproduces Figure 7: Equilibrium step-height fraction (SR), as a function of discharge Q, for four bed slopes.
`Figure_8.m`	Reproduces Figure 8: total, segment and step CO_2 outgassing as a function of discharge Q and bed slope.

3 Software requirements

- MATLAB (developed/tested with R2021b or later; earlier versions should work but are untested).
- **Statistics and Machine Learning Toolbox** — required for `poissrnd`, `exprnd`, `quantile`, `smoothdata`.
- **Optimization Toolbox** — required for `fsolve` in `CalculateDICfromCO2TA.m`.

4 Model inputs (`Data.m`)

Key entries of the input structure `I`, set in `Data.m`:

Field	Description	Units
`I.latitude`	Site latitude (Valfredda catchment)	degrees
`I.length`	Reach length	m
`I.slope0`	Mean bed slope	m/m
`I.ALK_0`, `I.ALK_L`	Upstream / lateral alkalinity	mol/m^3
`I.pCO2`	Upstream/lateral pCO_2	atm
`I.NEP`	Net ecosystem productivity	mol m^{-2} s^{-1}
`I.space_step`	Spatial discretization step	m
`I.T_water`	Water temperature	°C
`I.p_atm`	Atmospheric pressure at site elevation	atm
`I.Q`	Upstream discharge	m^3/s
`I.Ks`, `I.eta`	Gauckler–Strickler roughness coefficient and Manning exponent	$m^{\frac{1}{3}}/s$
fraction_steps	Fraction of total elevation drop assigned to discrete steps	0–1 (dimensionless)
`I.scenario`	Morphology scenario: 0 = homogeneous reach, 1 = single step, 2 = stochastic step field	—

5 Model outputs (`steady_state.m` → structure `O`)

For each spatial node along the reach, the output structure `O` contains: `O.DIC`, `O.ALK`, `O.pH`, `O.CO2`, `O.HCO3`, `O.CO3` (concentrations, mol/m^3), `O.FCO2` (areal evasion flux, mol m^{-2} s^{-1}), `O.JUMP_EVASION` (mass evaded at each step, mol/s), `O.eD` (energy dissipation rate, m^2/s^3), `O.k600` (gas transfer velocity, m/d).

6 How to reproduce the results

All scripts assume every `.m` file listed in Section 2 is on the MATLAB path (simplest: keep them all in one folder and `cd` into it, or run `addpath(genpath('path_to_repo'))`).

Figure 6

Run `Figure_6.m`. It sweeps discharge (`Q_values`, 15 log-spaced points from 10^{-3} to 10 m^3/s) and bed slope (`i_values` = 0.005, 0.01, 0.1) and, for each combination, runs stochastic realizations across `fraction_steps` = 0 to 0.99. Output: a plot of the relative change in total evaded CO_2 mass (step-dominated vs. step-free) as a function of Q, for each slope.

Figure 7

Run `Figure_7.m`. Same sweep structure as Figure 6, but with four slopes (0.005, 0.01, 0.05, 0.1), and the diagnostic computed is the step-height fraction (SR) that equalizes segment and step evasion. Output: semi-log plot of equilibrium SR vs. Q.

Figure 8

Run `Figure_8.m`. It sweeps `Q_values` (25 points) and `i_values` (0.005, 0.01, 0.05, 0.1) with `sim = 25` realizations per combination (no `fraction_steps` loop — a single stochastic step configuration per run). Outputs: (i) normalized morphological ratio W/λ_S vs. Q; (ii) median total/segment/step CO_2 outgassing vs. Q, one figure per slope.

Mass-balance check / flux decomposition

Run `DIC_model.m`. It runs `sim = 1000` realizations across `fraction_steps` = 0 to 0.99 and produces: evaded mass vs. normalized step height (percentile bands), a DIC mass-balance check (`balance_DIC`), and bar charts decomposing the DIC and CO_2 budgets into upstream/downstream/lateral, NEP, segment evasion, step evasion and carbonate-buffering terms.

7 Notes on reproducibility

The step configuration (number, position and height of steps) is generated stochastically in `Data.m` via a Poisson process (`poissrnd`) with exponentially distributed step heights (`exprnd`). Results therefore vary between runs unless a random seed is fixed. To obtain deterministic, byte-identical output for the archived version of the figures, add `rng(<seed>)` at the top of each driver script (`DIC_model.m`, `Figure_6.m`, `Figure_7.m`, `Figure_8.m`) before the simulation loop, and report the chosen seed here.