Local analysis of the gas exchange in a step-and-pool configuration via numerical simulation

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ABSTRACT

1. Introduction

Despite their small surface area, mountain streams are a significant source of greenhouse gases by efficient exchange processes at the water-air interface. The physical mechanisms responsible for the gas emission are modulated by the microtopography that characterizes the stream bed, whose steps and pools are peculiar examples (Botter et al., 2022). While it is well established that the gas transfer in correspondence with riverbed drops is promoted by the concurrence of high turbulence and bubble entrainment, a deep knowledge of the physical processes driving the outgassing dynamics in local steps still lacking. This study aims to bridge this knowledge gap by reproducing numerically the hydrodynamics of an idealized step-and-pool configuration.

2. Methods

The hydrodynamics of a step-and-pool configuration of a 0.3 m width rectangular section was simulated by the software Flow-3D Hydro 2022R1, and consisted in a broad-crested weir and a tapered positive step of height 25 and 9 cm, respectively, placed at a distance of 1 m. The limited pool has then a depth, z_0, of about 10 cm and is fed by a small cascade of almost 15 cm. The grid had nearly 7.5 million structured orthogonal cells. We solved the Reynolds-Averaged Navier-Stokes equations coupled with the re-normalization group e_k-ε scheme, e_k and ε being respectively the turbulent kinetic energy per unit of mass and the turbulent kinetic energy dissipation rate. Further, Flow-3D included the bubble entrainment due to the water flow according to the standard Advection-Diffusion Equation of a scalar of concentration C. Here, the air bubbles were assumed as spheres with a radius, r, of 0.5 mm. The model estimated both all the relevant hydrodynamic quantities and the entrained air concentration and escaping bubbles flux across the free surface, q_B. We set steady inflow of 2.0 l/s upstream of the weir, free outflow downstream of the step, and no-slip condition on both the bottom and channel sides. Initially, fluid was at rest, and the transient was less than 20 seconds before achieving the stationary solution. The results were preliminary assessed with data collected in a similar in-flume experiment.

3. Theory

The exchange of volumetric gas, F, through the water-air interface is described by the Henry's law as

$$F = k\left(C_w - \frac{C_a}{K_H}\right), \quad (1)$$

with k the gas transfer velocity, C_w and C_a the gas concentration in water and atmosphere, respectively, and K_H the Henry constant of the specific gas. In the present problem, k is due to the sum of the contributions induced by the turbulence, k_T, and the bubble mediated process, k_B, i.e., $k=k_T+k_B$. The eddies generated by the turbulence continuously exposed different portion of the water to the atmosphere, increasing k_T according to

$$k_T = \alpha_T Sc^{-0.5}(\nu\varepsilon)^{0.25}, \quad (2)$$

where α_T=0.2-0.4 is a coefficient, $\nu \approx 1\ 10^{-6}$ m^2/s is the kinematic viscosity of water, and $Sc=\nu/D$ is the Schmidt number, which expresses the link between kinematic and molecular diffusivity, D. Here, k_T was calculated using the computed value of ε near the free surface and assuming α_T=0.4 and the standard value of Sc= 600. The bubble-mediated process accounts the gas exchange between water and bubbles as long as they last in the water column. The exchange velocity, k_B, is proportional to the bubble flux according to

$$k_B = q_B\left(1 - e^{-T_B/T_g}\right)/\beta, \tag{3}$$

with β the Ostwald coefficient. $T_B \approx z_0/u_B$ (u_B the bubble rising velocity) is the bubble life time and $T_g(D, r, u_B)$ is the time scale of the gas transfer process (see Klaus et al., 2022). In this case, k_B was estimated for the CO_2.

4. Results and Discussion

In the pool, the cascade dissipates its energy through the local production and the subsequent dissipation of turbulent kinetic energy. The turbulence depletes indicatively 20% of the flow energy near the surface within a length that does not exceed a few centimeters near the cascade with consequent peak values of k_T of about 100 m/d (Fig. 1a). In addition, the falling jet is responsible for the entrapment of the air in the pool. The air bubbles extend for almost 30 cm downstream of the jet, but most of the air escaped in the first 10 cm, where k_B achieves a local maximum of about 500 m/d in small spots of 10 dm^2 (Fig. 1b). We compared the two mechanisms of gas evasion by the transverse-averaged values of the mass transfer rate $\bar{k}_T$ and $\bar{k}_B$ (Fig. 1c). The transfer velocity driven by the bubble-mediated process is almost one order of magnitude larger than that controlled by the turbulence in the central portion of the entrained air region. Accordingly, the outgassing in this region can be equivalent to the amount caused exclusively by the turbulence along some meters of the reach, which may be longer than the average two-next-steps distance in the headwaters.

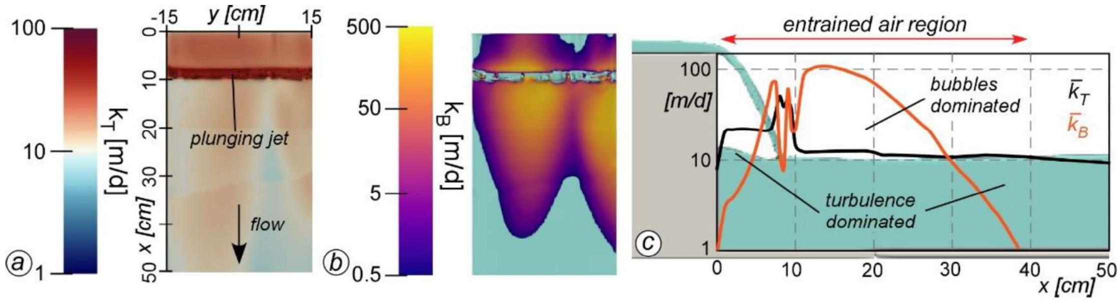

Fig. 1. Gas evasion in the pool. a) Field of k_T. b) Field of k_B. c) Transverse-averaged values of k_T and k_B. Adapted from Peruzzo et al. (2023).

Although direct transposition of the results to real-world scenarios requires caution, our simulation suggests that most of the observed gas evasion in mountain streams is likely bubble-mediated. The results raises two concerns about the correct procedure to quantify k in the stream. First, in this circumstance, k should be standardized not only in terms of Sc but also of β(and D), in particular, if tracer gases with different solubilities are used. Second, to correctly define an upscaling law between k and ε, as found in the literature (see, Ulseth et al., 2019), one needs to include the spatial frequency of steps and the relative contribution of the bubbles.

5. Conclusions

The present numerical analysis investigates the spatial patterns of energy dissipation and gas exchange, as well as the characteristic length scales of turbulence-induced and bubble-mediated gas transport in a step-and-pool configuration. According to the results, the gas evasion in the pool may be a very local process, taking place in a few dm^2 close to the plunging jet. Accordingly, aggregating k across heterogeneous reaches might be inherently biased (Botter et al., 2021), and k should be used with caution. In these cases, the mass transfer rate could be highly site-specific, and its extrapolation could be possible only through a detailed analysis of the evasion produced by the constitutive geomorphic elements of the reach. The outcomes may have significant implications in biology and environmental sciences that rely on correctly modeling gas cycles, such as CO_2.

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