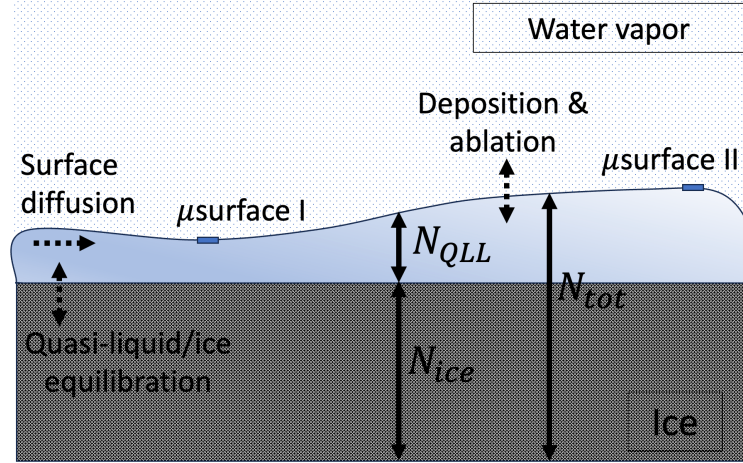


Figure 1. Visual representation of mesoscale variables N_{tot} , N_{ice} , and N_{QLL} , and processes affecting them, in QLC-1 (as well as the present revision, QLC-2) model. Dashed arrows represent processes affecting how these variables evolve over time.



QLC-2: A revised quasi-liquid reaction-diffusion model

Like QLC-1, QLC-2 represents an ice surface as two mesoscale variables and three processes, as shown in Fig. 1. The governing equations are

$$\frac{dN_{tot}}{dt} = D_{QLL} \nabla^2 N_{QLL} + v_{kin} \sigma_m \quad (1a)$$

$$\frac{dN_{QLL}}{dt} = \frac{dN_{tot}}{dt} - (N_{QLL} - N_{QLL}^{eq}(N_{tot}))/\tau_{eq} \quad (1b)$$

Some notes about this model are as follows, with differences between it and QLC-1 noted:

- 1) $D_{QLL} \nabla^2 N_{QLL}$ represents surface diffusion of the QLL; the underlying ice is considered immobile on time scales considered here.
- 2) v_{kin} is the rate at which vapor-phase water molecules strike the quasi-liquid; it is assumed that these stick with 100% efficiency, and thermalize on a picosecond time scale (i.e., instantaneously within the time scales of a QLC-2 simulation).
- 3) $N_{QLL}^{eq}(N_{tot})$ prescribes the thickness of quasi-liquid when it is in equilibrium with the underlying ice, according to

$$N_{QLL}^{eq}(N_{tot}) = \bar{N} - N^* \sin(2\pi N_{tot}) \quad (2)$$

This formulation ensures that the QLL thickness varies continuously from the thin microstate (“ μ surface I”) with thickness $\bar{N} - N^*$, to the thick microstate (“ μ surface II”) with thickness $\bar{N} + N^*$. (Note the connection to work of (Benet et al. 2019, Eq. 8), that also shows a sinusoidal dependence.)

- 4) Because μ surfaces I and II have different volatilities, the surface supersaturation at a given point on the surface (designated σ_m in Eq. 1a) is a function of both the microstate and the

water vapor concentration above it. To compute σ_m , we define a variable m that quantifies the degree to which a given surface is similar to μ surface I or II,

$$m = \frac{N_{QLL} - (\bar{N} - N^*)}{2N^*} \quad (3)$$

With this definition, μ surface I will have $m = 0$, while μ surface II will have $m = 1$. We then express the surface supersaturation as

$$\sigma_m(x) = \sigma_I(x) - m\sigma^o \quad (4)$$

where σ^o is a measure of the difference in the equilibrium vapor pressure of μ surfaces I and II, and $\sigma_I(x)$ is the supersaturation relative to μ surface I, mentioned previously. We will assume here that both σ^o (a scalar quantity) and $\sigma_I(x)$ are fixed parameters of a given solution. Eq. 4 is at slight variance with, and simpler than, the corresponding expression in QLC-1.

- 5) Typically, a parabolic form is used to approximate $\sigma_I(x)$ appearing in Eq. 4,

$$\sigma_I(x) \approx \sigma_{I,corner} \times \left(c_r \left(\frac{x}{L} \right)^2 + (1 - c_r) \right) \quad (5)$$

where c_r is a “center reduction”, the fractional reduction of supersaturation at facet centers relative to facet corners,

$$c_r = 1 - \frac{\sigma_{I,middle}}{\sigma_{I,corner}} \quad (6)$$

Negative values of c_r are also used in the simulations presented here, to represent the enhancement of water vapor concentration at facet centers when a crystal is ablating because of exposure to subsaturated conditions.

- 6) τ_{eq} is a first-order relaxation constant describing the time scale at which quasi-liquid/ice equilibrium is achieved. That is, if we imagine a surface with quasi-liquid amount N_{QLL}^o , then equilibration after a time Δt occurs according to

$$N_{QLL}(t) = N_{QLL}^{eq}(N_{tot}) + \left(N_{QLL}^o - N_{QLL}^{eq}(N_{tot}) \right) e^{-\frac{\Delta t}{\tau_{eq}}} \quad (7)$$

If one takes the time derivative of Eq. 6, and assumes that Δt is small, the second term on the right-hand side of Eq. 1b results.