APPENDIX A

The general equation describing oxygen transport through the lens-corneal system, in one dimension, is Fick's second law with reaction.[34]

$$k(x)\frac{\partial p(x,t)}{\partial t} = \frac{\partial}{\partial x}\left(k(x)D(x)\frac{\partial p(x,t)}{\partial x}\right) - Q(p(x,t)) \qquad \text{(Eq. A1)}$$

where p is the oxygen partial pressure in the lens-corneal system, t is time and x is the coordinate for normal cornea, with x=0 in the interface between the anterior chamber and the cornea.

The second term on the right-hand side in Eq. A1 is the oxygen consumption as a function of the partial pressure, which is absent in the contact lens and tears film regions and follows a Monod kinetics form in the corneal system:

$$Q_c(p_c) = \frac{Q_{c,\max} \cdot p_c(x)}{(K_m + p_c(x))} \qquad \text{(Eq. A2)}$$

In Eq. A1, solubility (k) and the diffusion coefficient (D) are considered as a function of the position, taking constant values across each of the two regions (CL and cornea) in the system. By using the above approach, we could obtain the complete pressure profile, provided that the continuity of the pressure is satisfied in the lens-corneal interface. This is automatically satisfied within our numerical scheme.

We chose the standard Dirichlet boundary conditions in the spatial coordinate:

$$P(t,0) = P_{ac} \quad and \quad P(t, x = L_c + L_{tears} + L_{lens}) = P_{air} \qquad \text{(Eq. A3)}$$

where P_{air} is the open-eye pressure, corresponding to the atmospheric pressure, and P_{ac} is the oxygen pressure in the anterior chamber.

As for the initial condition, we need to feed the stationary pressure profile in Eq. (1) in order to reproduce the evolution of the pressure profile from the closed-eye condition. This stationary closed-eye profile can be obtained by solving the steady-state equation:

$$\frac{\partial}{\partial x}\left(k(x)D(x)\frac{\partial P_{est}(x)}{\partial x}\right)-Q(P_{est}(x))=0 \qquad \text{(Eq. A4)}$$

which is obtained from Eq. A1 by removing the temporal evolution. Eq. A4 is subjected to the boundary conditions:

$$P_{est}(0)=P_{ac} \text{ and } P_{est}(x=L_c+L)=P_{PC}\,, \qquad \text{(Eq. A5)}$$

where P_{PC} is the contact-lens/palpebral conjunctiva oxygen pressure (*P_{PC}=61.4 mmHg)*.

We then used the solution to Eqs. A4-5 to define:

$$P(0,x)=P_{est}(x) \qquad \text{(Eq. A6)}$$

as the last boundary condition for Eq. A1).

The system of Eqs. A4-5 and Eqs. A1-3 and A6 are solved using FiPy,[45] a finite volume PDE solver written in Python. Table I shows the different values for the parameters used in the numerical solution of the equations. We used a spatial grid with 10^3 points in all computations and time steps of 10^{-1}s for the time-dependent equations.

First, Eqs. A4-5 are numerically solved and the resulting profile is used as initial condition for Eqs.1-3 and 6. An iterative procedure was used due to the nonlinear nature of the transport equations A1 to A6, by “sweeping” the solutions over few iterations (see FiPy manual for details http://www.ctcms.nist.gov/fipy). Convergence was reached after the residual was below a predefined value (10^{-11} in our case). We checked both grid size and time step parameters so that further decrease in size would not result in any improvement. All the computations were performed in a personal computer with an Intel Core i7-3770K under Debian Linux. FiPy version 3.0 was used in all computations.

Multidimensional parameter optimization subject to bounds was done through the “fmin_tnc” function in the Scipy package (http://www.scipy.org/), which uses a Newton Conjugate-Gradient method. We used this optimization procedure to determine the optimized values of $Q_{c,max}$ and K_m parameters in the Monod kinetics model, Q*, D_c and k_c in the Larrea et al. model,[22] and Q’ and k’ in the MMM, for a predefined set of remaining parameters in the model.