8. Computational Investigation of Ion Transport and Selectivity in Zwitterionic Hydrogel Membranes

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Abstract

Zwitterionic hydrogel membranes offer a distinctive route to ion-selective transport because cationic and anionic fixed groups coexist in a water-swollen polymer network. Their selectivity is not a simple function of net charge; it emerges from coupling among acid-base equilibria, Donnan partitioning, dielectric exclusion, hindered diffusion, and swelling. This manuscript develops a computational framework for ion transport and selectivity in such membranes. The model combines the Poisson-Nernst-Planck equations with a pH-dependent fixed-charge representation of zwitterionic sites, an interfacial Donnan equilibrium that includes dielectric and specific free-energy penalties, and a swelling condition that enforces osmotic, elastic, and ionic pressure balance. The formulation is discretized with a stabilized finite element method and treated as a coupled nonlinear system, with attention to boundary layers, electroneutrality assumptions, and parameter sensitivity. Analytical limits identify the dimensionless groups that control performance and clarify when a local Donnan model is adequate and when full diffuse-charge coupling is required. The analysis shows that net fixed charge governs co-ion exclusion, but the isoelectric condition does not eliminate selectivity because dielectric and mobility contrasts can remain. Divalent ions amplify both Donnan and dielectric effects, whereas swelling dilutes fixed charge and can offset gains in fixed-charge density. The framework provides a defensible basis for interpreting pH-responsive selectivity and for designing zwitterionic hydrogel membranes with controlled charge composition, crosslink density, and hydration.

Keywords

ion transport; zwitterionic hydrogels; Donnan equilibrium; Poisson-Nernst-Planck; membrane selectivity; dielectric exclusion

1. Introduction

Zwitterionic hydrogel membranes are crosslinked polymer networks that contain both cationic and anionic groups and retain substantial water within their pores. This composition makes them attractive for separations, sensors, electrochemical devices, and biointerfaces because hydration can be maintained while charge selectivity is tuned through copolymer composition and pH. The central design question is not whether such a membrane carries a net charge but how acid-base equilibria, Donnan partitioning, dielectric contrast, swelling, and ion valence combine to determine the partition and mobility of each species. Classical membrane equilibria provide the starting point for this problem through the Donnan description of charged interfaces [1]. Fixed-charge ion-exchange theory then supplies the relationship between charge density, counterion enrichment, and co-ion exclusion [2], while electrodiffusion theory describes how concentration and potential gradients produce coupled ionic fluxes [3,4].

Continuum models of charged membranes are commonly built from electrochemical potential gradients and mass conservation [5]. When convection is present, the same framework is extended through convective-diffusive transport relations and hydrodynamic boundary conditions [6]. For zwitterionic hydrogels, however, the charged groups are not inert. Protonation and deprotonation change the net fixed charge, and the local environment can produce dielectric and hydration effects that are not captured by a single charge-density parameter. Zwitterionic materials are known for strong hydration and resistance to nonspecific adsorption [7], and their functional derivatives have been developed for applications that require controlled interfacial behavior [8]. These properties motivate a computational treatment that resolves both the equilibrium partitioning of ions and the transport limitations imposed by the polymer network.

Polymer swelling introduces an additional coupling that is often absent from rigid-pore membrane models. The equilibrium volume of a hydrogel reflects a balance among mixing, elastic, and ionic osmotic contributions [9], and gel swelling theories provide the classical formalism for relating these contributions to polymer volume fraction and crosslink density [10]. Because ion partitioning changes the ionic osmotic pressure, swelling modifies fixed-charge density and porosity, which in turn modify ion transport. A computational model that treats fixed charge and porosity as constants can therefore miss an important feedback mechanism in zwitterionic membranes.

Charged interfaces and thin double layers also impose numerical and conceptual constraints. Diffuse-charge dynamics in electrochemical systems can depart substantially from local electroneutrality when double layers are comparable to the system size or when transient currents are applied [11]. The Nernst-Planck equation has well-known limits in membrane systems, particularly when interfacial kinetics, finite ion size, or strong correlations become important [12]. Dielectric exclusion provides one route beyond simple Donnan theory by penalizing ions that enter a low-permittivity polymer phase [13]. Steric, electric, and dielectric exclusion models have been developed for nanofiltration membranes [14,15], and hindered transport theory describes how pore confinement reduces effective diffusivities [16]. General diffusion theory and double-layer descriptions provide the surrounding physical background [17,18], while colloidal electrostatics and polymer physics supply the necessary relations for charged soft materials [19,20].

This manuscript contributes a computational framework that treats these couplings explicitly rather than folding them into an empirical selectivity coefficient. The framework retains Poisson coupling instead of assuming electroneutrality everywhere, represents the zwitterionic fixed charge through pH-dependent site equilibria, incorporates an interfacial Donnan condition with dielectric and specific free-energy penalties, and closes the system with a swelling equilibrium. The analysis below derives the governing equations, describes a numerically stable solution strategy, and uses limiting cases to identify the conditions under which Donnan exclusion, dielectric exclusion, or mobility contrast dominates. The aim is to provide a technically defensible basis for interpreting ion transport in zwitterionic hydrogel membranes and for selecting charge composition, crosslink density, and hydration as design variables.

2. Computational Framework

2.1. State variables and governing equations

Consider a membrane domain and adjacent electrolyte reservoirs separated by interfaces. The mobile species include salt cations, salt anions, hydrogen ions, and hydroxide ions. Multivalent ions can be added without changing the structure of the model. The unknown fields are the concentration of each mobile species, the electric potential, the polymer volume fraction, and the pressure. The flux of species i is written as

$$J_i \;=\; -\,D_i\,(\nabla c_i \;+\; z_i\,F/(RT)\,c_i\,\nabla\varphi) \;+\; c_i\,u$$

where J_i is the molar flux, D_i is the effective diffusivity, c_i is the concentration, z_i is the valence, F is Faraday's constant, R is the gas constant, T is temperature, φ is the electric potential, and u is the solvent velocity. The first term combines diffusion and migration in the Nernst-Planck form, while the final term represents convective transport. The effective diffusivity is allowed to depend on polymer volume fraction so that hindered transport in the hydrogel can be represented [16]. The solvent velocity is obtained from a Darcy or Brinkman relation for the porous network; because the present analysis focuses on ion partitioning and electromigration, u is treated as a specified or separately coupled field.

Mass conservation for each mobile species gives

$$\partial c_i/\partial t \;=\; -\,\nabla\cdot J_i \;+\; R_i$$

where t is time and R_i is a source term. For inert salt ions, R_i is zero. For hydrogen and hydroxide ions, R_i includes acid-base reactions with the zwitterionic sites. When specific ion binding is included, the corresponding association and dissociation terms are added to R_i. The continuity equation is solved in both the membrane and the adjacent solution, with interfacial conditions enforcing flux continuity and local equilibrium where the interface is treated as infinitesimally thin.

The electric potential satisfies Poisson's equation,

$$-\nabla\cdot(\varepsilon\,\nabla\varphi) \;=\; F(\textstyle\sum_i z_i\,c_i \;+\; \rho_f)$$

where ε is the position-dependent permittivity and ρ_f is the fixed charge density of the polymer network. The permittivity is written as ε = ε_0 ε_r(φ_p), where ε_0 is the vacuum permittivity, ε_r is the relative permittivity, and φ_p is the polymer volume fraction. Poisson's equation is retained rather than replaced by electroneutrality because double layers can be comparable to pore dimensions, especially at low ionic strength, near the isoelectric point, or during transient charging [11]. The fixed charge density is not constant in a zwitterionic hydrogel. It is determined by the protonation state of the cationic and anionic groups according to

$$\rho_f = Fc_T\left[\frac{1}{\left(1+10^{pH-pK_a+}\right)}-\frac{1}{\left(1+10^{pK_a--pH}\right)}\right]$$

where c_T is the total concentration of zwitterionic sites per gel volume, pK_a+ characterizes the cationic group, and pK_a- characterizes the anionic group. The pH is defined from hydrogen ion activity. The first term represents the fraction of sites that are positively charged, and the second represents the fraction that are negatively charged. When the two fractions are equal, the net fixed charge vanishes at the isoelectric condition. Even at that condition, however, local positive and negative sites remain and can affect ion hydration, dielectric properties, and specific interactions.

2.2. Interfacial and swelling closures

At a membrane-solution interface, equality of electrochemical potentials for each mobile species yields a Donnan-type partition relation,

$$\ln\left(\frac{c_i^m}{c_i^s}\right) = -z_i F \Delta\frac{\varphi_D}{(RT)} - \Delta\frac{W_i}{(RT)}$$

where c_i^m and c_i^s are concentrations on the membrane and solution sides, Δφ_D is the Donnan potential difference, and ΔW_i is the excess free-energy penalty for transferring species i into the membrane environment. The term ΔW_i includes dielectric exclusion, steric exclusion, and any specific adsorption or hydration contribution. The partition coefficient is K_i = c_i^m/c_i^s. For an ideal Donnan model, ΔW_i is omitted. For a low-permittivity hydrogel, the Born penalty for a charged species increases with z_i^2 and with the inverse of its effective radius, so multivalent ions can be strongly excluded even when the net fixed charge is modest [13]. The interfacial condition can be imposed directly at a thin interface or recovered by solving Poisson's equation across an explicitly resolved diffuse layer.

The swelling equilibrium closes the coupling between ion partitioning and network deformation. It is expressed as

$$\Pi_m ix(\varphi_p) + \Pi_e l(\varphi_p) + RT\sum_i (c_i^m - c_i^s) = 0$$

where Π_mix is the mixing osmotic pressure, Π_el is the elastic osmotic pressure of the crosslinked network, and the final term is the ionic osmotic pressure. The sum over mobile species includes all ions that partition into the membrane. This relation follows from equality of solvent chemical potential between the gel and the external solution and is consistent with classical gel swelling theory [9,10]. The mixing and elastic terms depend on polymer volume fraction and crosslink density, while the ionic term depends on the charge state and external salt concentration. Consequently, a change in pH that alters ρ_f can change swelling, and a change in swelling can alter ρ_f through dilution of c_T.

The performance metric for ion selectivity is the permeability ratio,

$$\alpha_i j = \left(\frac{P_i}{P_j}\right) = \frac{(D_i K_i)}{(D_j K_j)}$$

where P_i is the effective permeability of species i, D_i is its effective diffusivity in the membrane, and K_i is its partition coefficient. For a steady one-dimensional membrane of fixed thickness, P_i is proportional to D_i K_i divided by an effective transport length. The selectivity α_ij is therefore a product of a mobility ratio and a partition ratio. A membrane can be highly selective in equilibrium partitioning but still show modest permeability selectivity if the more strongly partitioned ion diffuses much more slowly.

Under the simplifying conditions of ideal partitioning, constant diffusivities, and no specific binding, substitution of the Donnan relation into the permeability ratio gives

$$\alpha_i j = \left(\frac{D_i}{D_j}\right)\exp\left[-(z_i - z_j)F\Delta\frac{\varphi_D}{(RT)} - \frac{(\Delta W_i - \Delta W_j)}{(RT)}\right]$$

This expression separates the contribution of charge valence and Donnan potential from the contribution of excess free-energy penalties and mobility. It is useful for sensitivity analysis because it shows that selectivity between ions of different valence is exponential in

the Donnan potential, whereas selectivity between ions of the same valence is controlled primarily by ΔW_i differences and mobility. The expression also makes clear that a vanishing net fixed charge does not necessarily produce α_{ij} equal to unity when dielectric or specific interactions differ between species.

3. Numerical Implementation and Computational Workflow

The coupled system formed by the flux, continuity, Poisson, fixed-charge, Donnan, and swelling relations is nonlinear and spatially stiff. A finite element discretization is natural because the membrane geometry, interfaces, and electrode boundaries can be represented without forcing a one-dimensional approximation. The concentration and potential fields are approximated on a mesh that is refined near the membrane-solution interfaces, where concentration and potential gradients are steep. The polymer volume fraction can be treated as an element-wise or continuous field depending on whether swelling is allowed to vary spatially. When a thin-interface Donnan condition is used, the interface is represented by a boundary condition; when diffuse charge is to be resolved explicitly, the membrane and solution are meshed together and Poisson's equation is solved across both domains.

The transport equations require stabilization when the Péclet number based on solvent velocity or electromigration is large. A standard Galerkin formulation can produce oscillatory concentrations and negative values that are physically inadmissible. Streamline upwind Petrov-Galerkin stabilization or an exponential-fitting scheme related to the Scharfetter-Gummel discretization can be used to preserve monotonicity in one-dimensional limits. The Poisson equation is coupled to the transport equations through the charge density and through the permittivity dependence on polymer volume fraction. A monolithic Newton-Krylov solver with a block preconditioner is often effective because the coupling between concentration and potential is strong. Alternatively, a Picard iteration between transport and Poisson can be used when the nonlinearity is mild, but convergence is less reliable near limiting-current conditions.

Time integration is required when transient charging, step changes in applied potential, or changes in reservoir composition are of interest. Implicit Euler or a variable-order backward differentiation formula avoids the severe time-step restriction associated with explicit treatment of diffusion. The time step is adapted according to local truncation error and Newton convergence. For steady-state problems, the time derivative is omitted and the Newton iteration is applied directly to the nonlinear algebraic system. In either case, mass balance is checked for each mobile species, and the total current is verified against the applied current or potential condition.

Boundary conditions must be chosen to match the experimental or device configuration. At reservoir boundaries, concentrations are fixed or related to electrode reactions. At electrodes, either the potential or the current density is specified. At symmetry planes, zero normal flux and zero normal electric field are imposed. The polymer network is confined to the membrane, so the polymer volume fraction has zero normal flux at the membrane boundaries. If the interface is treated as infinitesimally thin, the Donnan relation supplies the jump in concentration and potential; if the interface is resolved, no such jump condition is imposed and the diffuse layer emerges from the Poisson equation. The former is computationally efficient but assumes local equilibrium and a double layer much thinner than the membrane. The latter is more demanding but is required when double-layer thickness is comparable to pore size or when the applied potential varies rapidly.

Verification of such a solver relies on mesh refinement, conservation checks, and comparison with independent limiting solutions. In the limit of zero fixed charge and zero excess free energy, the model should reduce to ordinary electrolyte transport. In the limit of a thin double layer and high salt concentration, it should reproduce the local Donnan model. In the limit of negligible transport, it should recover the equilibrium Donnan partition and swelling relation. Common failure modes include unresolved boundary layers, Newton divergence caused by strong exclusion and near-zero concentrations, artificial charge accumulation at interfaces, and violation of mass balance when the flux discretization is not conservative. These failure modes are not peripheral numerical details; they determine whether the computed selectivity can be trusted.

4. Analytical Assessment of Selectivity Mechanisms

For a membrane with net fixed charge, the Donnan relation in Eq. 5 already indicates the basic trend: co-ions are excluded and counterions are enriched. The exponent is linear in z_i, so divalent co-ions experience approximately twice the Donnan potential of monovalent co-ions under otherwise comparable conditions. A modest net fixed charge can therefore produce a large separation between monovalent and divalent ions. This is the classical basis of Donnan selectivity [1,2]. The same relation shows why selectivity falls as the external salt concentration increases: the Donnan potential is screened by the mobile ions, and the partition coefficients approach unity when the fixed charge is small relative to the total ionic strength. In the language of diffuse-charge theory, the Debye length becomes small compared with the membrane thickness, and local electroneutrality becomes an accurate approximation away from the interfaces [11].

Zwitterionic membranes complicate this picture because the net fixed charge is pH-dependent. Equation 4 expresses ρ_f as the difference between the positively charged and negatively charged site fractions. At a pH below both pK_a values, the cationic groups are largely protonated and the net charge is positive; at a pH above both values, the anionic groups are largely deprotonated and the net charge is negative. Near the isoelectric condition, the two fractions cancel and ρ_f is small. A naive interpretation would conclude that Donnan selectivity disappears at that point. The more complete model shows that this is not necessarily true. The local positive and negative sites remain, and the excess free-energy term ΔW_i in Eq. 5 can differ between ions because of size, hydration, and dielectric contrast. Dielectric exclusion is especially important for multivalent ions because the Born penalty scales with z_i^2. Thus, a membrane near its isoelectric point can still discriminate ions through dielectric and specific interactions even when net charge exclusion is weak [13,15].

Swelling introduces a feedback that can either reinforce or oppose selectivity. Equation 6 shows that an increase in ionic osmotic pressure tends to swell the network. Swelling dilutes the total site concentration c_T and therefore reduces the magnitude of ρ_f for a given degree of protonation. It also increases the water content and pore size, which generally raises effective diffusivities. The net effect on permeability is therefore a competition between weaker Donnan exclusion and faster diffusion. If the target separation depends on co-ion exclusion, excessive swelling is detrimental. If the target separation depends on mobility contrast, moderate swelling may be beneficial. Crosslink density is the principal design variable that sets this trade-off because it controls the elastic osmotic pressure and the maximum swelling extent.

Mobility contrast is the second factor in Eq. 8. Even when partition coefficients differ strongly, the permeability ratio can be compressed by differences in D_i. Hindered transport

in a polymer network reduces D_i for larger ions and for ions that interact strongly with the polymer [16]. The effective diffusivity also depends on porosity, tortuosity, and the spatial distribution of polymer chains. For this reason, a selectivity calculation that uses bulk solution diffusivities can overestimate the permeability of the more strongly partitioned species. The computational framework treats D_i as a function of polymer volume fraction and, when necessary, of local composition. This is preferable to absorbing mobility effects into an apparent partition coefficient because it keeps the equilibrium and transport contributions separately interpretable.

Transient operation adds another layer. When a current is applied, concentration polarization develops at the membrane-solution interfaces, and the local ionic strength can differ from the reservoir value. Diffuse-charge dynamics can produce transient potentials that are not predicted by electroneutral models [11]. At high current density, the system can approach a limiting current, beyond which water splitting or other electrode reactions dominate. In a zwitterionic hydrogel, the limiting current can be modified by the buffering action of the acid-base sites and by the swelling response to local ionic strength. These effects are captured by the coupled Poisson-Nernst-Planck formulation but not by a fixed-charge, electroneutral Donnan model. The practical implication is that selectivity measured under equilibrium partitioning may differ from selectivity observed under current flow, especially for thin membranes or low-salt conditions.

The dimensionless groups that govern these regimes follow directly from the equations. The ratio of Debye length to membrane thickness determines whether diffuse charge must be resolved explicitly. The Péclet number based on solvent velocity or electromigration determines whether convective or migrative terms produce sharp boundary layers. The ratio of fixed charge density to bulk ionic strength determines the strength of Donnan exclusion. The ratio of excess free-energy penalty to thermal energy determines the importance of dielectric exclusion. These groups are not independent: swelling changes fixed charge density and porosity, pH changes fixed charge and possibly the permittivity, and ionic strength changes both screening and osmotic pressure. A sensitivity analysis should therefore vary them jointly rather than one at a time.

5. Technical Discussion and Design Implications

The framework supports several design inferences. First, net fixed charge is the primary lever for monovalent-versus-divalent selectivity when Donnan exclusion dominates. A high fixed-charge density favors strong co-ion exclusion, but it also increases ionic osmotic pressure and swelling, which dilutes the charge. The optimal charge density is therefore not necessarily the maximum achievable value; it is the value at which Donnan exclusion remains strong without driving the network into an over-swollen state. Crosslink density can be used to limit swelling, but excessive crosslinking reduces porosity and effective diffusivity, which can lower permeability and sharpen concentration polarization. The design problem is thus a constrained trade-off among selectivity, permeability, and mechanical stability.

Second, the pH response of zwitterionic groups provides a route to tunable selectivity that is not available in fixed-charge membranes. By choosing pK_a values that are separated and by controlling the ratio of cationic to anionic sites, a membrane can be made positive, neutral, or negative over a useful pH range. The isoelectric condition is not a selectivity dead zone if dielectric or specific interactions are present, but it is a point at which Donnan control is weak and the membrane becomes more sensitive to ion size, hydration, and specific binding. This sensitivity can be exploited for separations that require discrimination among ions of the same

valence, but it also makes the membrane vulnerable to small changes in pH or ionic composition. Computational screening of pK_a spacing and site ratio is therefore more informative than treating pH as a single operating variable.

Third, dielectric contrast can dominate selectivity for multivalent ions. If the polymer phase has a lower relative permittivity than the external solution, the Born penalty for transferring an ion into the membrane increases with z_i^2 and with inverse ion radius. This favors the exclusion of multivalent and small ions and can produce selectivity even when net fixed charge is small. The zwitterionic groups themselves are strongly hydrated, so the local permittivity is not simply that of the dry polymer. The dependence of ε_r on polymer volume fraction and on local ionic composition is a key input. A model that assumes a constant permittivity can misrepresent the balance between Donnan and dielectric exclusion, particularly near the isoelectric point.

Fourth, the coupling between swelling and transport means that selectivity is not a purely local property. A membrane that is selective in a thin surface layer can lose performance if the interior swells and provides a low-resistance pathway for co-ions. Conversely, a moderately swollen membrane can benefit from faster counterion diffusion if the partition selectivity is preserved. The spatial distribution of crosslink density, charge density, and polymer volume fraction therefore matters. The finite element formulation can represent graded membranes, but the design analysis should distinguish between surface-dominated and bulk-dominated selectivity. In thin membranes or high-flux operation, interfacial polarization and boundary layers can dominate the measured selectivity, so the intrinsic partition and mobility ratios may not be directly observable.

The model also clarifies the limits of simplified treatments. An electroneutral Donnan model is efficient and often adequate when the Debye length is much smaller than the membrane thickness and when the applied current is low. It becomes unreliable when double layers overlap, when the membrane is nanoporous, or when transient charging is important. A full Poisson-Nernst-Planck model resolves these effects but remains a mean-field description. Ion-ion correlations, finite ion size, dielectric saturation, and specific adsorption can become important at high valence and high concentration [19]. The present framework should therefore be understood as a bridge between molecular-level parameters and membrane-scale performance, not as a replacement for molecular simulation. Its value lies in making the coupling among charge equilibria, dielectric exclusion, swelling, and transport explicit and testable through sensitivity analysis.

6. Conclusion

This manuscript has formulated a computational framework for ion transport and selectivity in zwitterionic hydrogel membranes. The framework couples Poisson-Nernst-Planck transport with pH-dependent fixed charge, interfacial Donnan partitioning that includes dielectric and specific free-energy penalties, and a swelling equilibrium that links ionic osmotic pressure to polymer volume fraction. The resulting equations retain diffuse charge where it matters, represent the acid-base state of the zwitterionic sites explicitly, and separate equilibrium partitioning from mobility. Analytical limits show that net fixed charge controls Donnan exclusion, but the isoelectric condition does not eliminate selectivity because dielectric and mobility contrasts can remain. Divalent ions amplify both Donnan and dielectric effects, while swelling dilutes fixed charge and can offset gains in charge density. The numerical requirements are demanding because the system is nonlinear, stiff, and sensitive to boundary layers and interfacial conditions. Stabilized finite elements,

conservative flux discretization, adaptive meshing, and robust nonlinear solvers are therefore essential. The framework provides a technically grounded basis for interpreting pH-responsive ion selectivity and for designing zwitterionic hydrogel membranes through charge composition, crosslink density, and hydration, while also identifying where mean-field continuum treatment must be supplemented by molecular or correlation-aware descriptions.

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