Kirchhoff Coupling Generates ATP, the Chemical Energy of Life

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SUMMARY

Electrons flow. Voltages change in biology as in physics. Current — if it includes displacement current — moves according to Kirchhoff's law, on all scales. Current energizes devices and creates signals in biology as in engineering.

In biology, current flow creates chemical energy stored in the form of ATP (adenosine tri-phosphate) in mitochondria. ATP is the nearly exclusive source of chemical energy in life.

Kirchhoff's current law couples electron flow and proton movement in mitochondria, as our research group, led by Huaxiong Huang, has shown, see Fig. 1 and Ref. [1]. When they are coupled in membrane proteins, electron and proton fluxes form a device − in the strict engineering sense of the word − that produces ATP as an output. See [2] for meaning of biological names.

BACKGROUND

Atomic details control function in these protein devices. Atomic details must be included if models of proteins are to be useful in immensely important medical applications. Those atomic details are manipulated when treatments of disease and drugs are designed in hundreds or thousands of laboratories every day, by 'site directed mutagenesis'.[2]

Atomic details are difficult to include in models and simulations of proteins because biological systems include so many atoms ($>10^{18}$) that move quickly (10^{-15} sec), compared to biology ($>10^{-4}$ sec). Most of the quick motions are irrelevant to biological function but we do not yet have a method ('coarse graining') to reliably take advantage of that fact. Coarse graining of space is dangerous because it so easily hides the reality that a few atoms can control biological function in a quite specific way.

Biological function, including current flow, is thus difficult to compute in simulations with atomic resolution.

Fortunately, it is often not necessary to compute current flow with atomic resolution. Engineers rarely have to consider the atomic details of current flow in wires, for example. Biophysicists rarely have to consider the atomic details of current flow in their 'wires', the interior of long (meters), slender (μm) nerve cells.

Kirchhoff's current law makes it possible to study current without atomic detail in both engineering and biology. Current flow − if it includes displacement current − follows Kirchhoff's current law as implied by taking the divergence of the Maxwell Ampere law [3].

$$\mathbf{div}\left(\mathbf{curl\,B}\right) = \mathbf{div}\left(\overbrace{\mu_0\mathbf{J} + \mu_0\varepsilon_0\ \partial\mathbf{E}/\partial t}^{Total\ Current}\right) = 0;$$

$\mathbf{J}$ includes flux of **all** charges

Kirchhoff's current law is true on the atomic scale and on the macroscopic scale because Maxwell's equations work on both scales.

Kirchhoff's current law forces current flow in one component of the circuit to depend on current flow in another component. The different components can have entirely different mechanisms of current flow. The mechanism does not matter. The mechanism can vary, with time or conditions. It can depend on other fields, not included in the classical Maxwell equations. Total current is conserved in all cases. Kirchhoff's current law forces a relation between the currents, independent of the mechanism of the movement of electrons, ions, or other charges. Currents are coupled by the Maxwell equations and nothing else − not by chemical or atomic mechanisms. Kirchhoff coupling is as universal as the Maxwell equations themselves.

In particular, Kirchhoff's current law couples electron flow in cytochrome c oxidase to proton flow. Proton flow in turn generates ATP in another protein device, that is a synthase of ATP [2].

Without Kirchhoff's current law it would be difficult if not impossible to simulate or compute coupling of electron and proton flow. Without Kirchhoff's current law, it would be impossible to recognize the physical imperative that currents are coupled, even if currents flow in disjoint components, far separated with unrelated mechanisms, because of the Maxwell equations.

Kirchhoff's current law couples electron, proton, and ATP movements in mitochondria, and it couples electron and proton movements in the two different protein devices of cytochrome c oxidase and ATP synthase [2].

It is no wonder that molecular dynamics simulations of mitochondria have not identified coupling by current flow. The interactions of the $>10^{18}$ atoms that make up macroscopic current flow involve numbers far beyond what can be computed. Stirling's formula says that the number n of pairwise interactions of 10^{18} atoms is something like $n! \approx \left(10^{18}\right)^{\left(10^{18}\right)}$, and interactions in a Coulombic fluid are not just pairwise.

CONCLUSION

The laws of circuits are needed to understand the chemical energetics of life. Kirchhoff coupling creates one of the most important processes in life. Kirchhoff coupling of different chemical species is a general mechanism. Kirchhoff coupling generates ATP, a source of chemical energy. Although not widely used in molecular biology, Kirchhoff's current law is as important in biology as in engineering.

REFERENCES

[1] Xu, Eisenberg. Song, Huang. (2022) Mathematical Model for Chemical Reactions…in Cytochrome c Oxidase: Electro-osmotic Approach. Preprint arXiv:220702215.

[2] *Wikipedia* and *YouTube* provide excellent discussions and comforting visualizations of biological names like ATP, mitochondria, cytochrome c oxidase, ATP synthase, and site directed mutagenesis. 'Proton' is lab jargon for any positively charged form of water, e.g., H_3O^+ or $H_5O_2^+$.

[3] Eisenberg, Oriols, Ferry. Kirchhoff's Current Law with Displacement Current (2022). arXiv: 220708277.

Eisenberg. A Necessary Addition to Kirchhoff's Current Law of Circuits. (2022) EngArXiv. DOI: 10.31224/2234

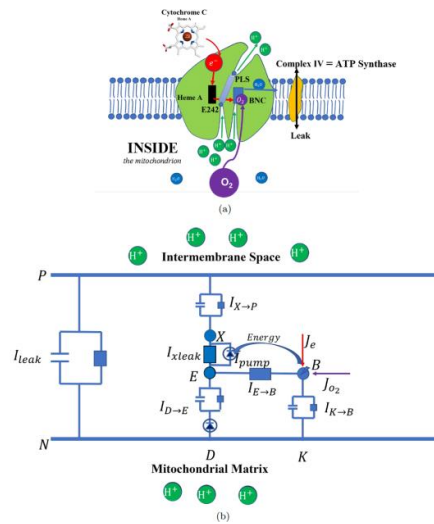**Fig. 1. Cytochrome C oxidase and Equivalent Circuit**

Fig. 2 Representative Result. Different Oxygen concentration. (a) Reaction rate; (b) Electron concentration _e; (c) [H]B; (d) [H]E; (e) [H]X. Dashed line − − computed from default parameters.