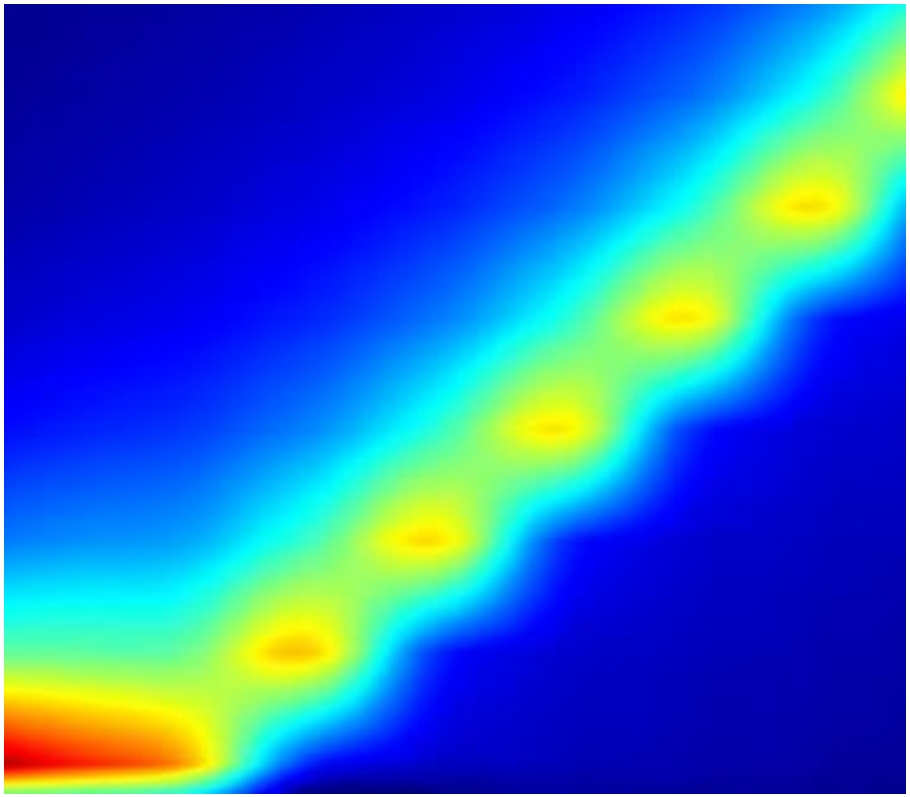


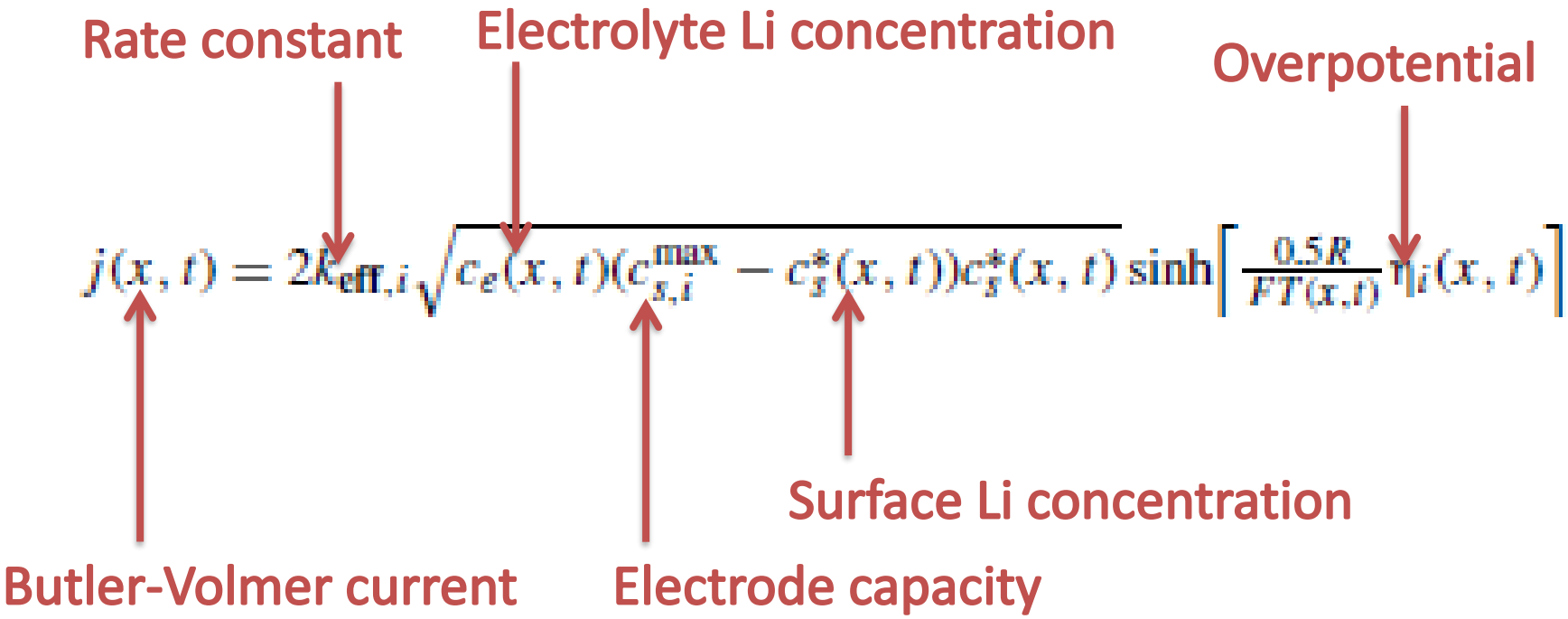
Spatio-temporal evolution of charge transfer current in an Li-ion battery

Charge Transfer Current

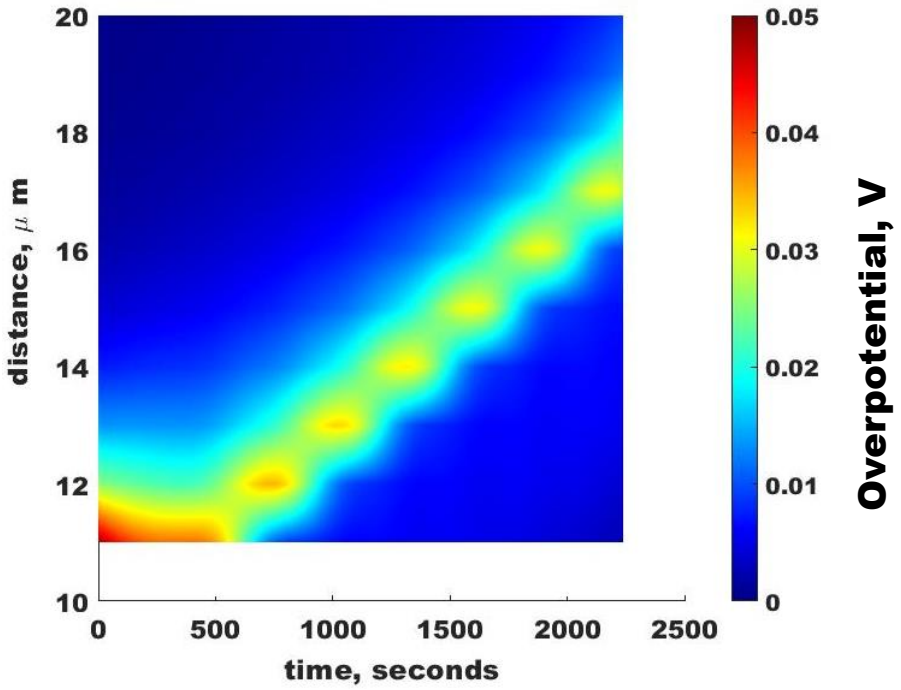
- Drives battery charge/discharge process
- Involves two parallel phenomena
  - Dissolution of Li_+ ions into electrolyte
  - Conduction of electrons through electrode material and carbon fillers

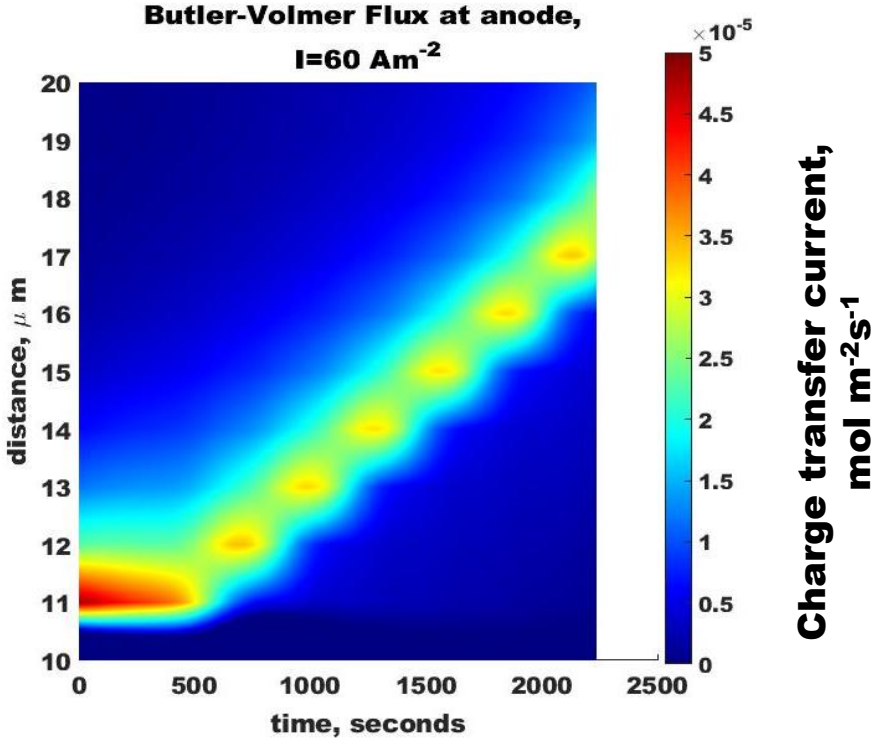
Representation

- Commonly used method: Butler-Volmer current
- Hypothesis:
  - Activation energy = weighted average of oxidized and reduced states



Factors driving spatio-temporal evolution



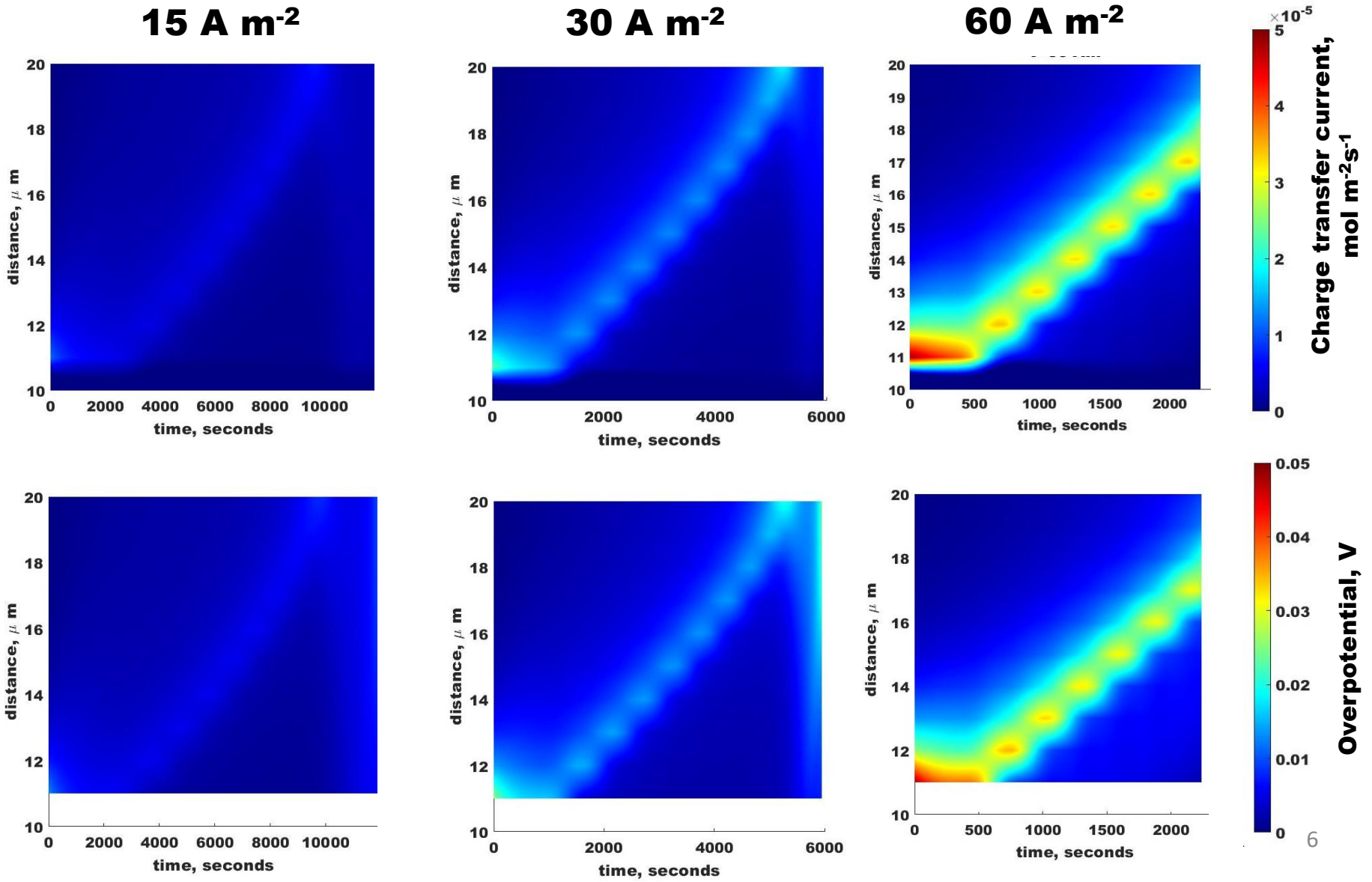


- LION-SIMBA 1-D P2D multiphysics model
  - Input current 60 A m^{-2}
  - T=298K
  - Graphite anode, $LiCoO_2$ cathode
- Marked correlation between Butler-Volmer flux and overpotential (ɳ)

Spatio-temporal evolution of overpotential

- Beginning of discharge: concentration polarization due to instantaneous charge transfer at the outermost layer (#10)
  - Lithium atoms from inner layers move in to fill in outermost layer
  - Surface lithium concentration, and hence potential, relaxes to its steady state, open circuit value
  - Outermost layer closest to separator, first to empty
- Phenomenon repeated over inner layers

How does applied current affect overpotential and charge transfer dynamics?



Key takeways

- Overpotential hotspots and consequently Butler-Volmer flux increase with applied current
- Highest overpotentials and fluxes for 60 A m^{-2}
  - Higher currents provide lesser relaxation time
- Lowest overpotentials and fluxes at 15 A m^{-2}
  - Attributed to ability to relax to open circuit value
- System for most of the time is at open circuit voltage for all 3 input currents