Niru Battery
Manufacturing Co.

University of
Tehran

One-Dimensional Modeling of Lead-Acid Batteries Using CFD

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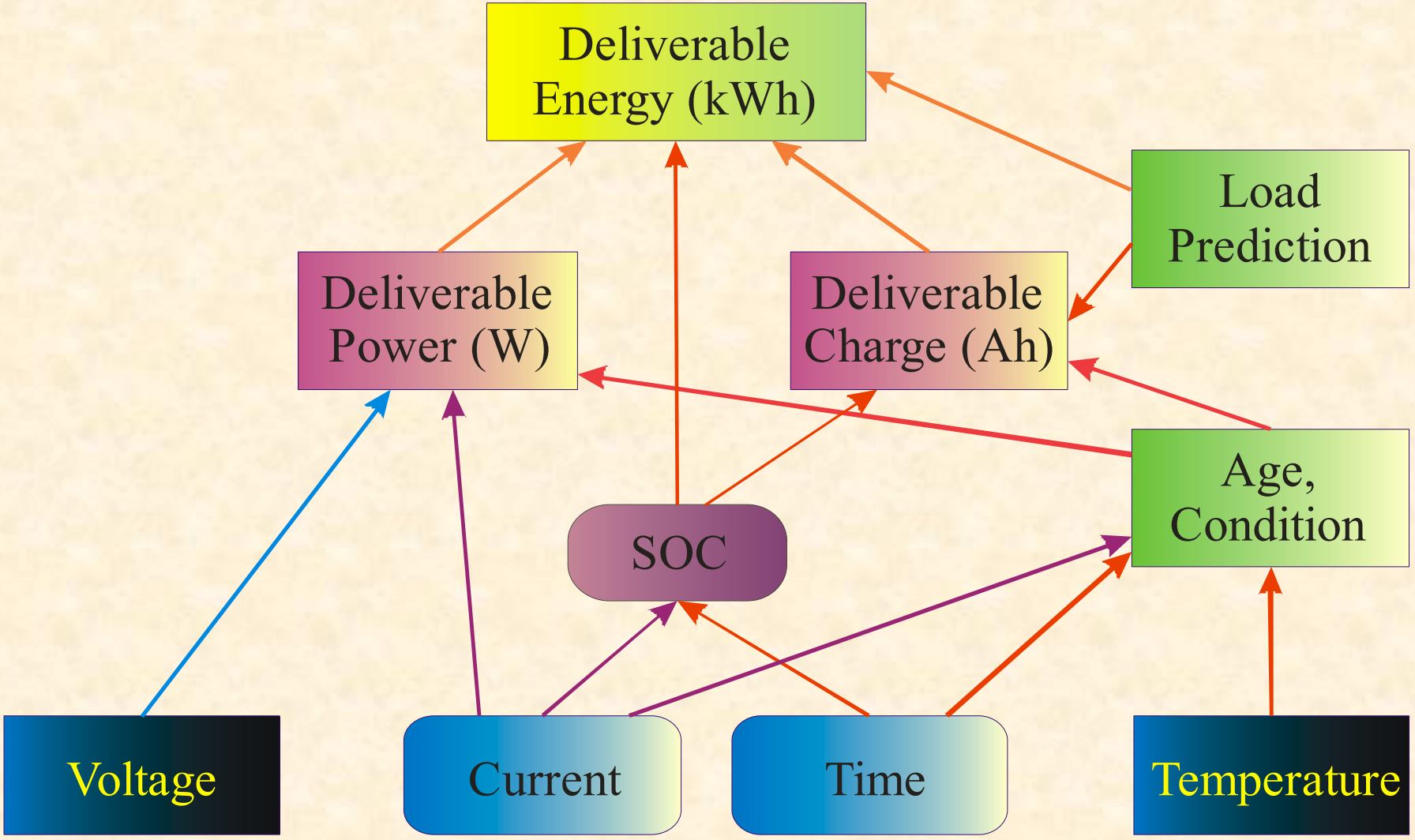
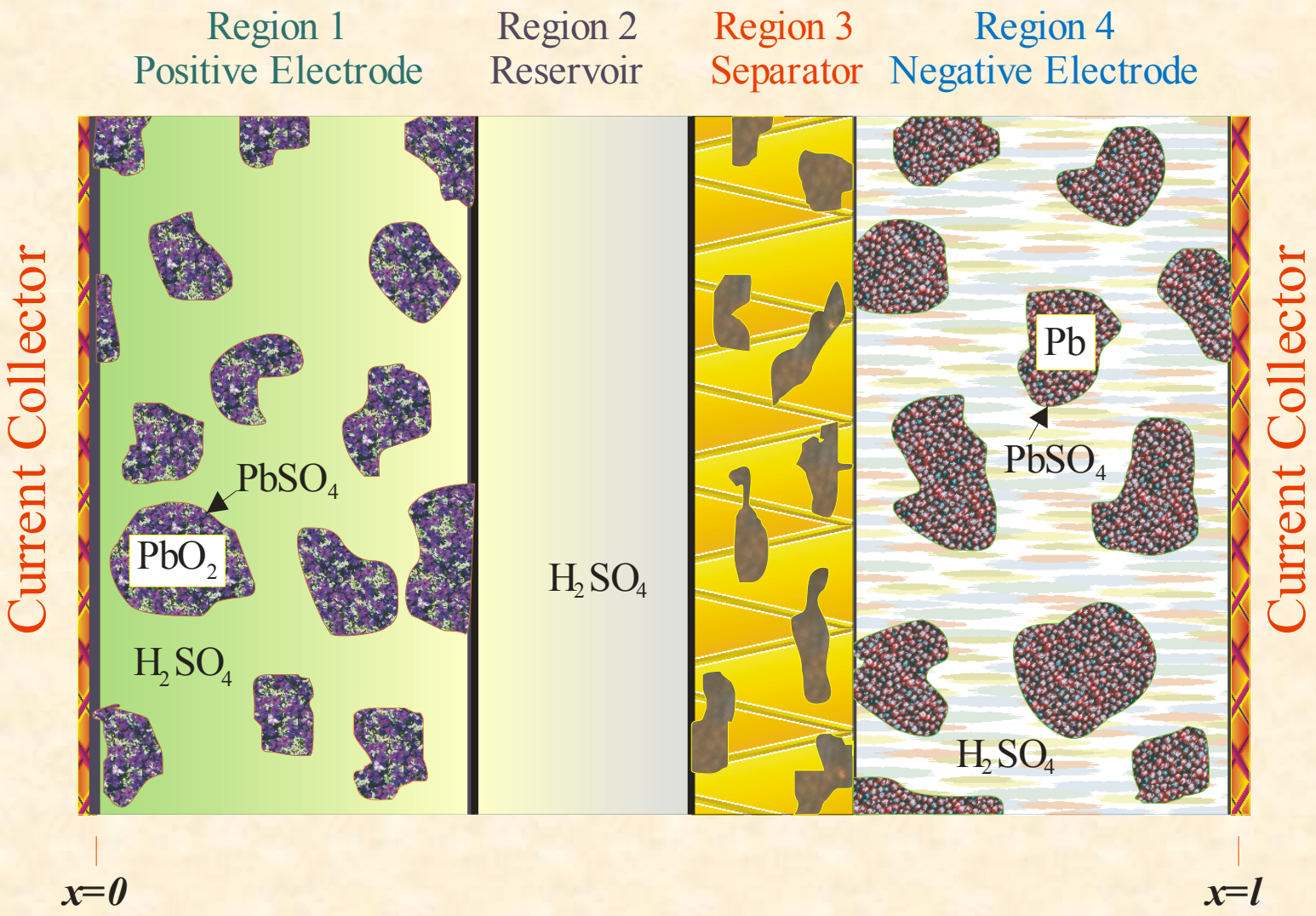
Why Modeling?



Methods of Modeling

- Dynamic Modeling
  - Based on equivalent circuit
  - Dynamic behavior of Battery
  - Requires many experimental data
  - Simulation of *TIME* dependant variables
- CFD Modeling
  - Stands for **C**omputational **F**luid **D**ynamics
  - Solving transport equations numerically
  - Simulation of battery in *TIME* and *SPACE*
  - CFD can provide *INPUTS* for dynamic modeling
  - Investigating the effect of different parameters on battery performance

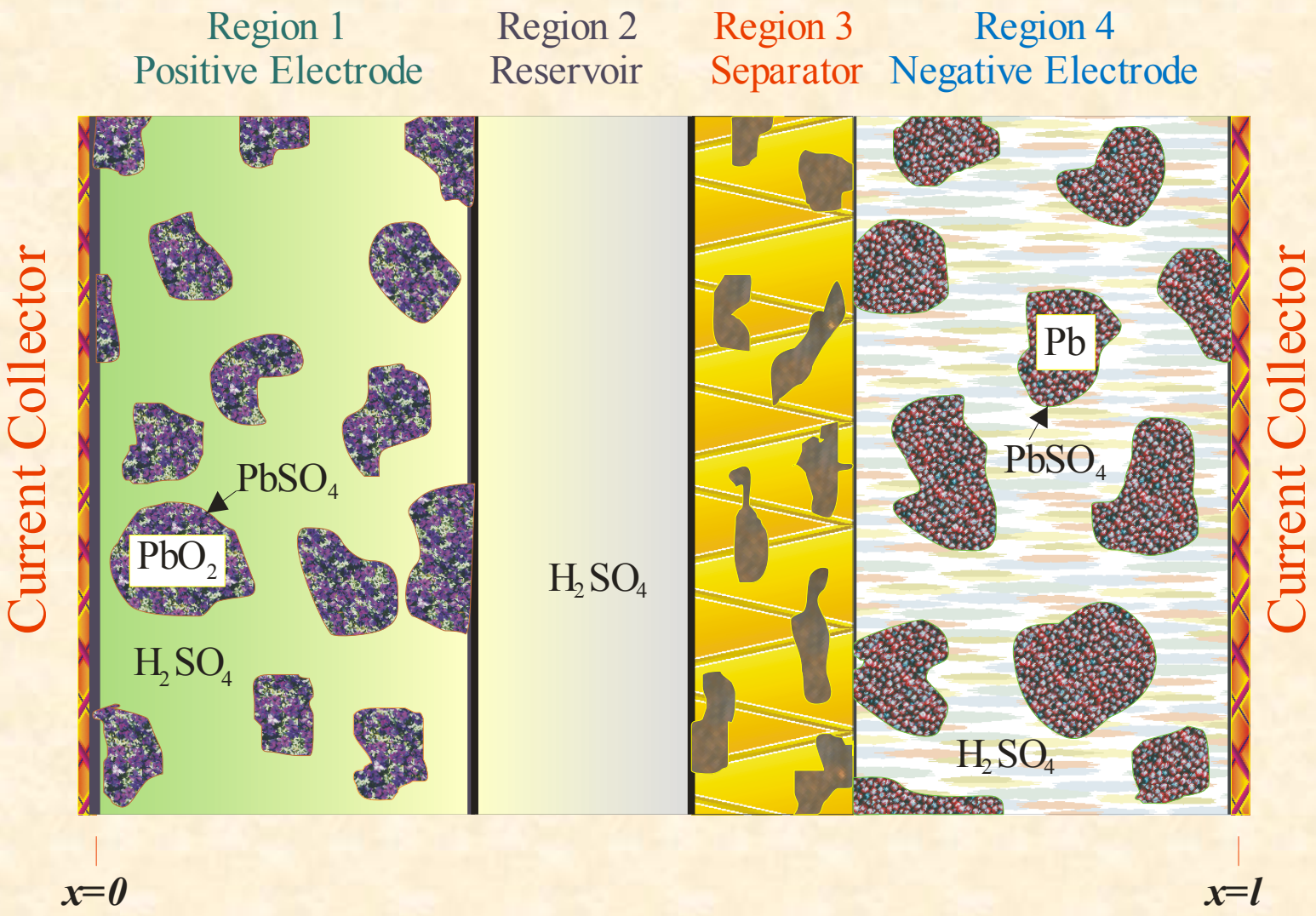
Lead-Acid Battery Model



History

- Hirman Gu et al. (1987)
  - Transport equations in each region
  - Requires matching conditions at boundaries
  - Off-diagonal blocks at boundaries
  - Using a special routine for off-diagonal blocks
  - Finite Difference Method
- W. B. Gu et al. (1997)
  - Integrated coupled electrochemical model
  - No need for matching conditions at boundaries
  - Finite Volume Method

Lead-Acid Battery Model



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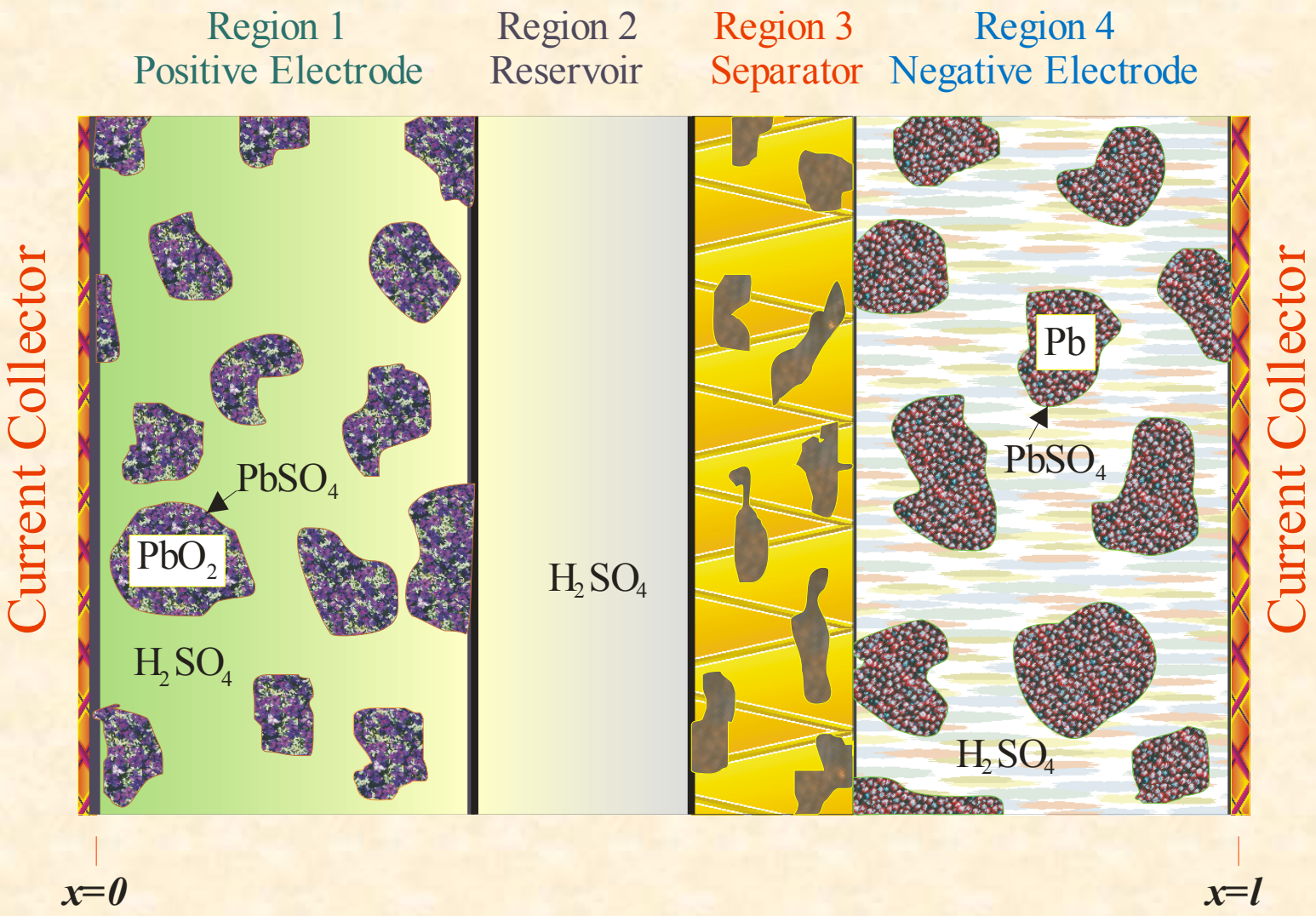

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Coupled Electrochemical and Transport Processes in Lead-Acid Batteries

– Conservation of Charge in Solid

$$\nabla \cdot (\sigma^{\text{eff}} \nabla \phi_s) - Aj = 0$$

– Conservation of Charge in Liquid

$$\nabla \cdot (k^{\text{eff}} \nabla \phi_l) + \nabla \cdot (k_D^{\text{eff}} \nabla (\ln c)) + Aj = 0$$

– Species (ionic) Conservation

$$\frac{\partial(\epsilon c)}{\partial t} + v \cdot \nabla c = \nabla \cdot (D^{\text{eff}} \nabla c) + a_2 \frac{Aj}{2F}$$

– Conservation of Momentum

$$\frac{\partial v}{\partial t} + v \cdot \nabla v = -\frac{1}{\rho} \nabla p + \nabla \cdot (\nu \nabla v) + g[1 + \beta(c - c_\circ)] + \frac{\nu}{K}(\epsilon v)$$

– Conservation of Mass

$$\nabla \cdot v = 0$$

One-Dimensional Assumptions

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0

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– Conservation of Mass

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Governing Equations (1-D)

– Conservation of Charge in Solid

$$\frac{\partial}{\partial x}\left(\sigma\frac{\partial \phi_s}{\partial x}\right) = +Aj$$

– Conservation of Charge in Liquid

$$\frac{\partial}{\partial x}\left(k\frac{\partial \phi_l}{\partial x}\right) = -Aj - \frac{\partial}{\partial x}\left(\frac{k}{c}\frac{\partial c}{\partial x}\right)$$

– Species (ionic) Conservation

$$\epsilon\frac{\partial c}{\partial t} = \frac{\partial}{\partial x}\left(D\frac{\partial c}{\partial x}\right) + a_2\frac{Aj}{2F} - c\frac{\partial \epsilon}{\partial t}$$

Boundary Conditions

- Potential in Solid

$$\phi_s = 0, V \qquad \text{or} \qquad -\sigma^{\text{eff}} \frac{\partial \phi_s}{\partial x} = I$$

- Potential in Liquid

$$\frac{\partial \phi_l}{\partial x} = 0$$

- Acid Concentration

$$\frac{\partial c}{\partial x} = 0$$

Initial Conditions

- Initial acid concentration

$$c = c_0$$

- Initial potential in solid and liquid

1. Solve steady state equations.

$$\frac{\partial}{\partial x}\left(\sigma \frac{\partial \phi_s}{\partial x}\right) = +Aj \quad \text{and} \quad \frac{\partial}{\partial x}\left(k \frac{\partial \phi_l}{\partial x}\right) = -Aj - \frac{\partial}{\partial x}\left(\frac{k}{c}\frac{\partial c}{\partial x}\right)$$

0

2. Solve the whole system up to a small time step (i.e. 10^{-4} sec.)

Numerical Difficulties

- All equations are highly non-linear
- Non-linear source terms

$$j = i_{\circ}\left(\frac{c}{c_{\mathrm{ref}}}\right)^{\gamma}\left\{\exp\left(\frac{\alpha_a F}{RT}(\phi_s - \phi_l - \Delta U_{\mathrm{PbO_2}})\right) - \exp\left(\frac{\alpha_c F}{RT}(\phi_s - \phi_l - \Delta U_{\mathrm{PbO_2}})\right)\right\}$$

- The system of equations is highly stiff
- All equations are highly coupled together
- All boundary conditions are of Newman type (singularity occurs)

Numerical Scheme

- Method of use: Keller-Box
- Specifications
  - Delta formulation
  - Implicit
  - 2^{nd}-order accurate in TIME and SPACE
- Advantages
  - Calculation of the functions and their derivative simultaneously
  - Leads to a block tridiagonal matrix
  - Can be used on nonuniform grid
  - Large band of stability
  - Ease of programming

Numerical Procedure

- Convert the system to first order system of Equations
- Linearization of the system
- Solve the system iteratively using Newton's iteration method

Converting to 1-st order System

- Defining

$$\frac{\partial \phi_s}{\partial x} = u$$

$$\frac{\partial \phi_l}{\partial x} = v$$

$$\frac{\partial c}{\partial x} = w$$

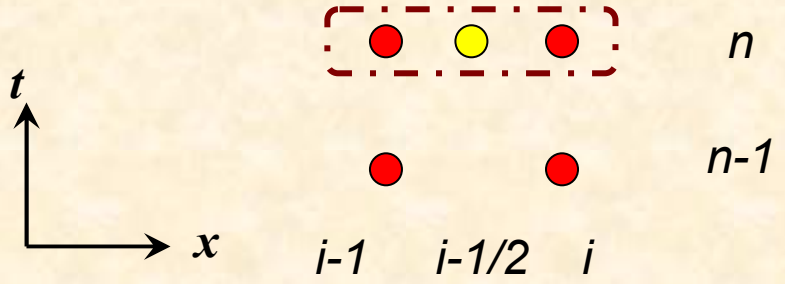
The System of Equations

- We have

$$
\begin{cases}
\dfrac{\partial(\sigma^{\text{eff}} u)}{\partial x} &= +Aj \\
\dfrac{\partial \phi_s}{\partial x} &= u \\
\dfrac{\partial(k^{\text{eff}} v)}{\partial x} &= -Aj - \dfrac{\partial}{\partial x}\left(\dfrac{kw}{c}\right) \\
\dfrac{\partial \phi_l}{\partial x} &= v \\
\epsilon \dfrac{\partial c}{\partial t} &= \dfrac{\partial(D^{\text{eff}} w)}{\partial x} + (a_2 - a_1 c)\dfrac{Aj}{2F} \\
\dfrac{\partial c}{\partial x} &= w
\end{cases}
$$

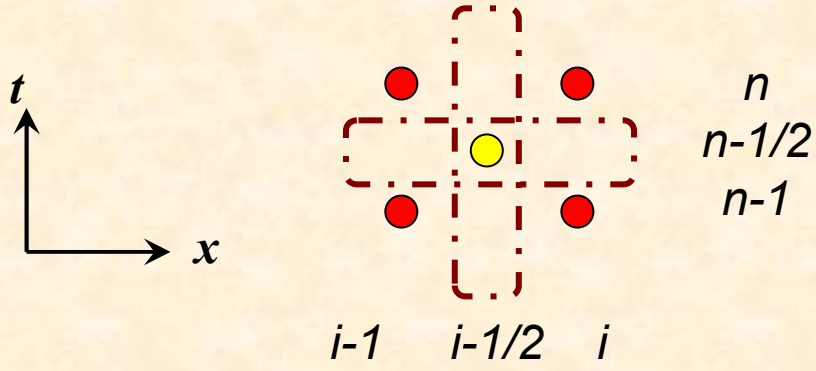
Discretization

- Time independent equations are differenced at location *i-1/2* and time level *n*



$$\left.\frac{\partial \Psi}{\partial x}\right|_{i-1/2}^{n} = \frac{\Psi_i^n - \Psi_{i-1}^n}{\Delta x_i}$$

- Time dependent equations are differenced at location *i-1/2* and time level *n-1/2*



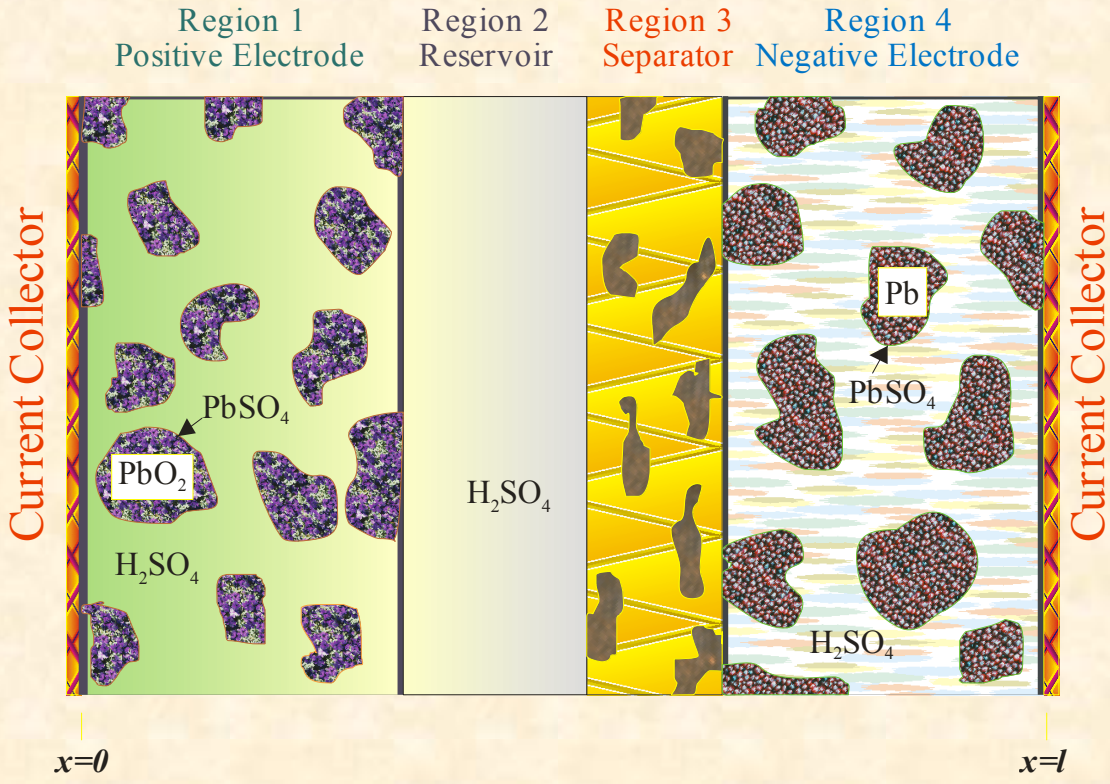
Block tridiagonal system

$$\begin{bmatrix} [B][C] & & \\ [A][B][C] & & \\ & \ddots & \\ & & [A][B] \end{bmatrix} \begin{bmatrix} [X_1] \\ [X_2] \\ [X_3] \\ \vdots \\ [X_n] \end{bmatrix} = \begin{bmatrix} [RHS_1] \\ [RHS_2] \\ [RHS_3] \\ \vdots \\ [RHS_n] \end{bmatrix}$$

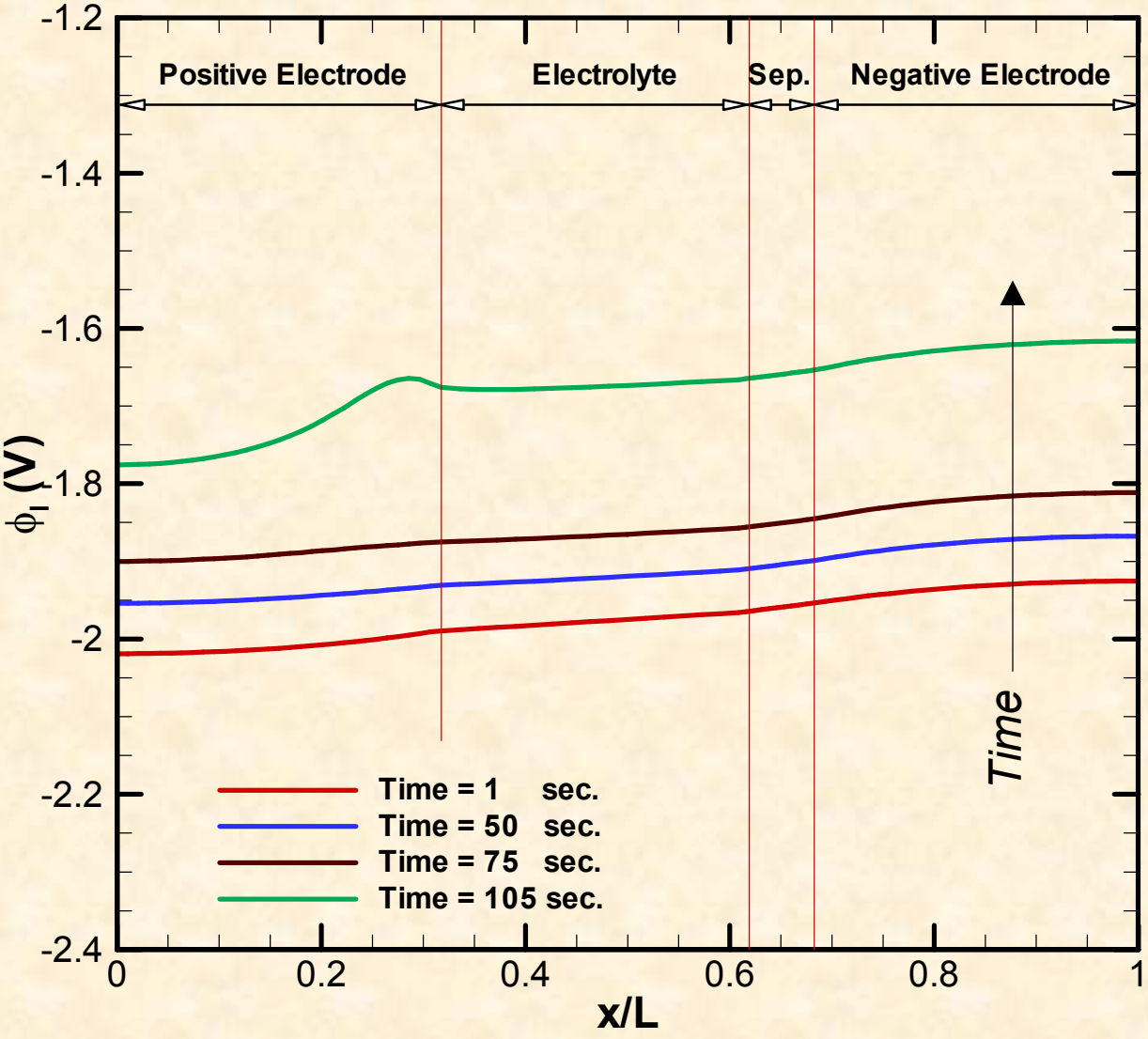
$$[X_n] = \begin{bmatrix} \delta \ \phi_s \\ \delta \dfrac{\partial \phi_s}{\partial x} \\ \delta \ \phi_l \\ \delta \dfrac{\partial \phi_l}{\partial x} \\ \delta \ c \\ \delta \dfrac{\partial c}{\partial x} \end{bmatrix}$$

Simulated Sample

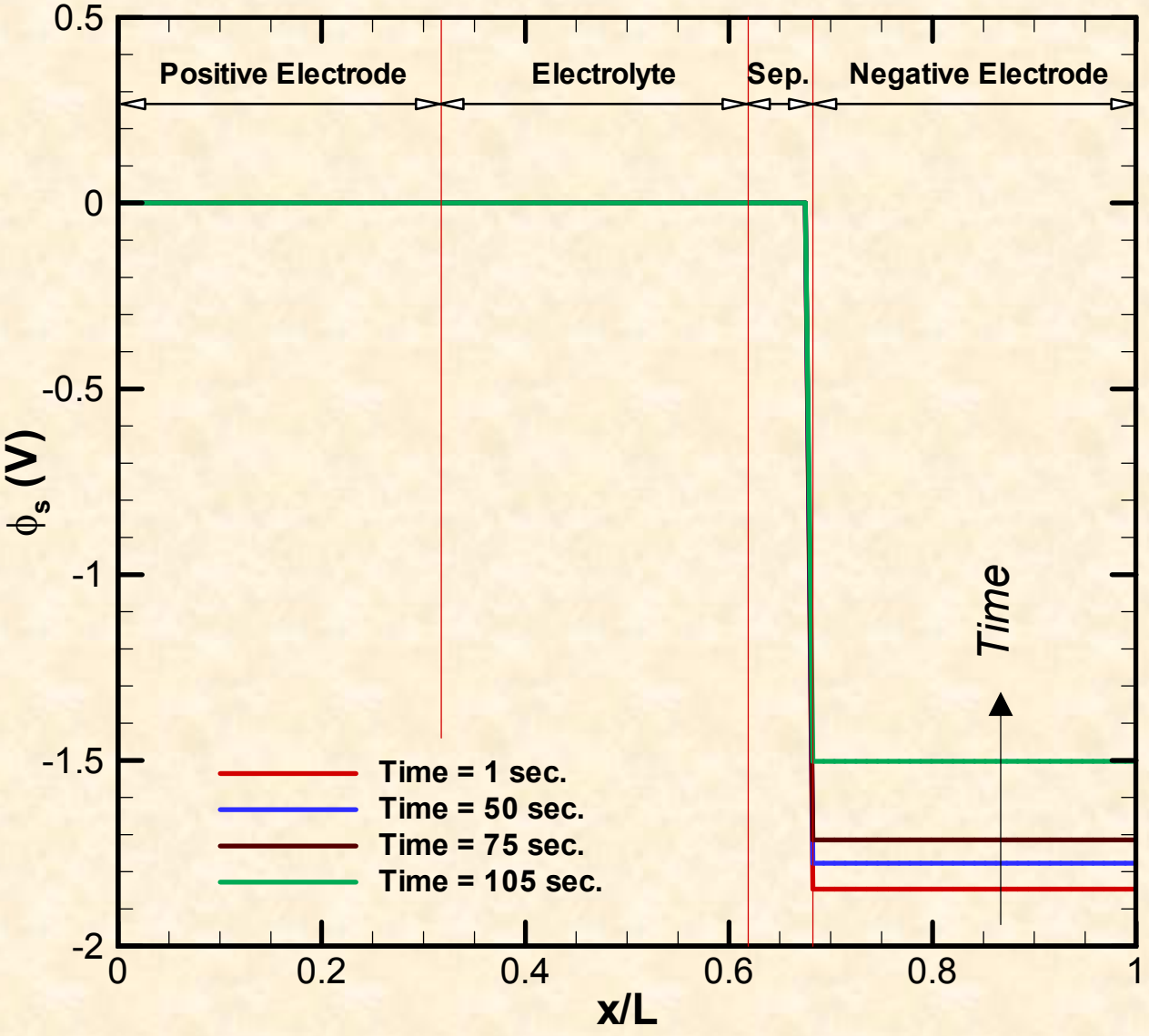
- H. Gu et al. (1987)
  - Discharge (*I=-340* mA)



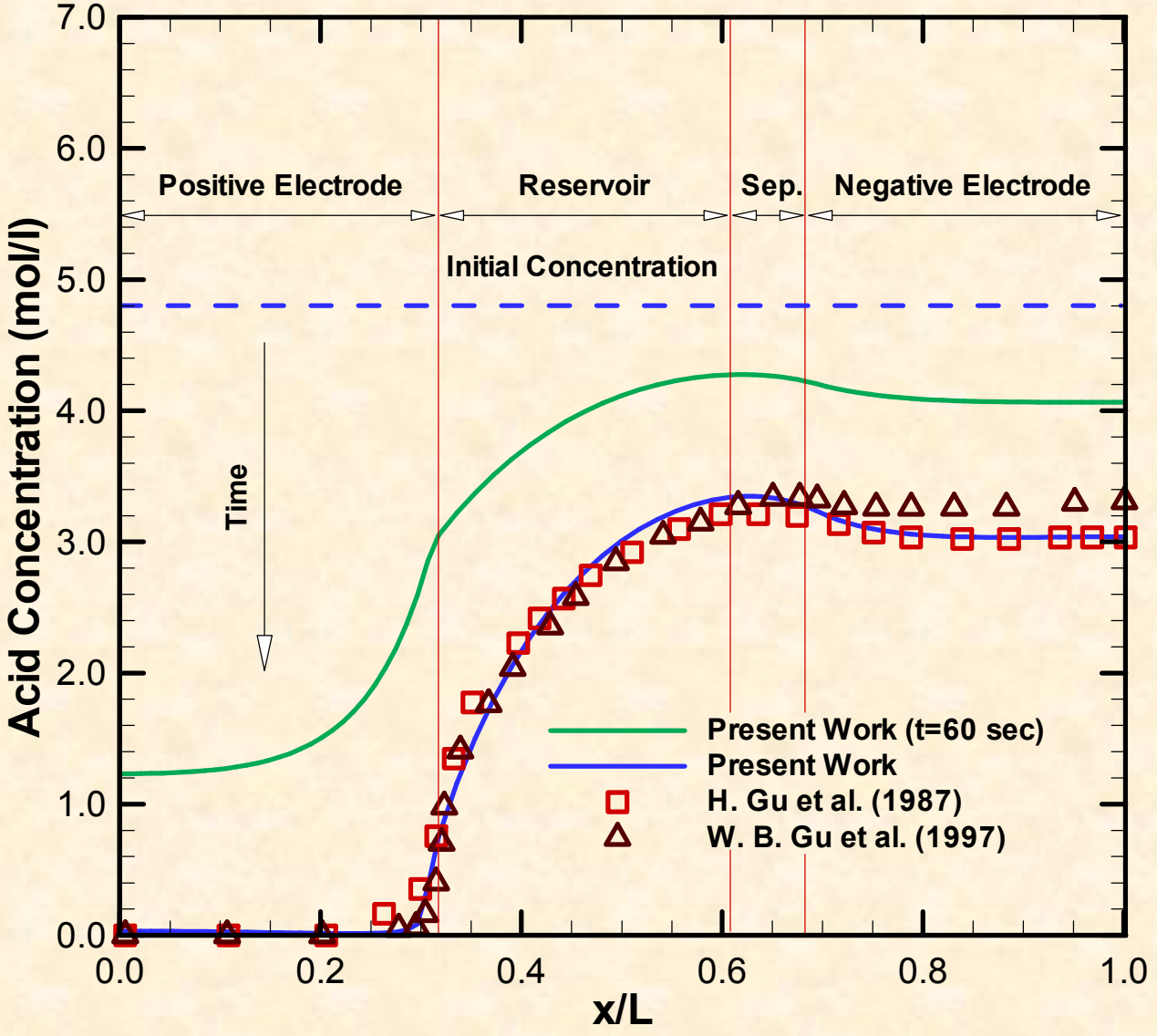
Potential in Liquid



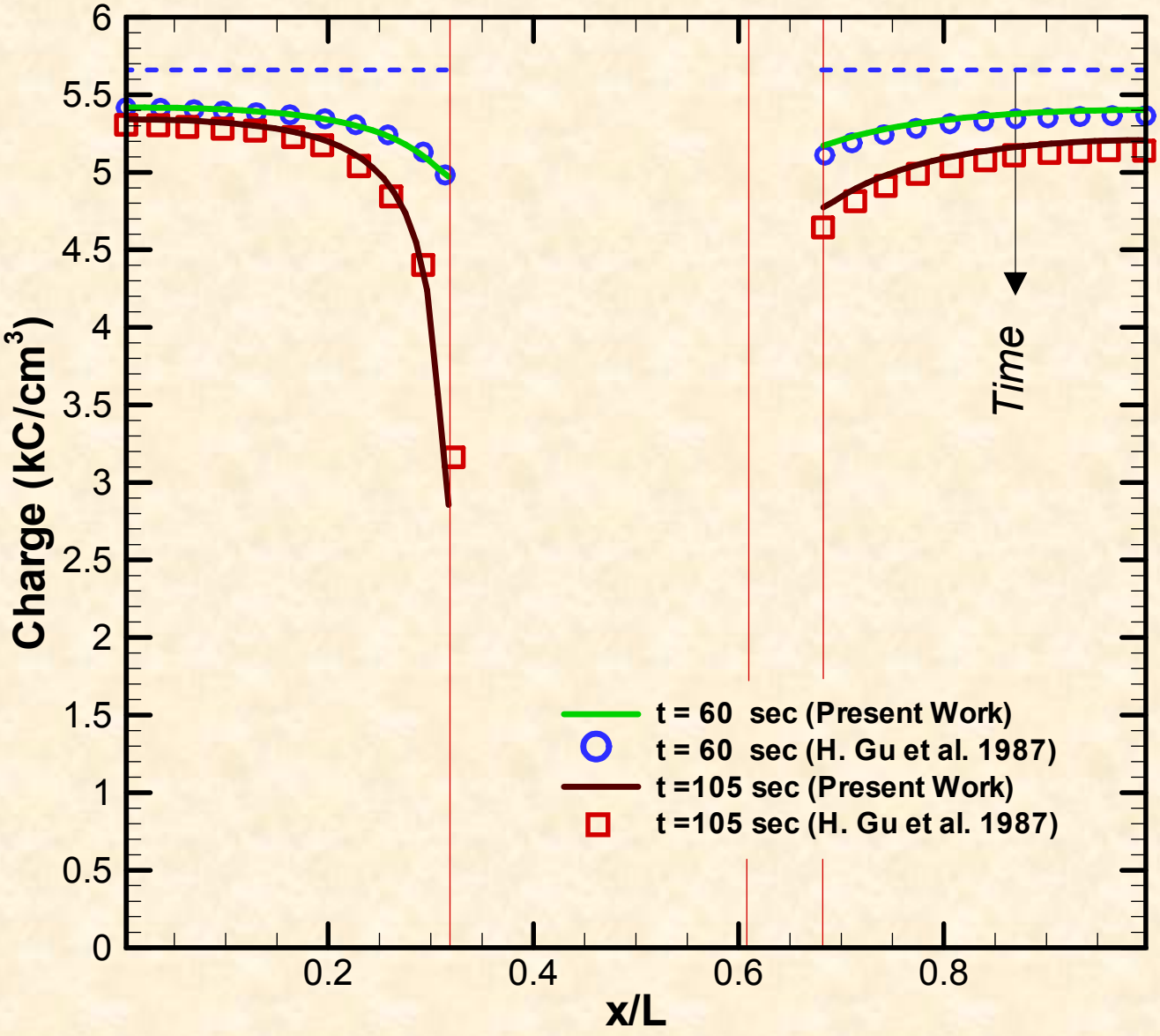
Potential in Solid



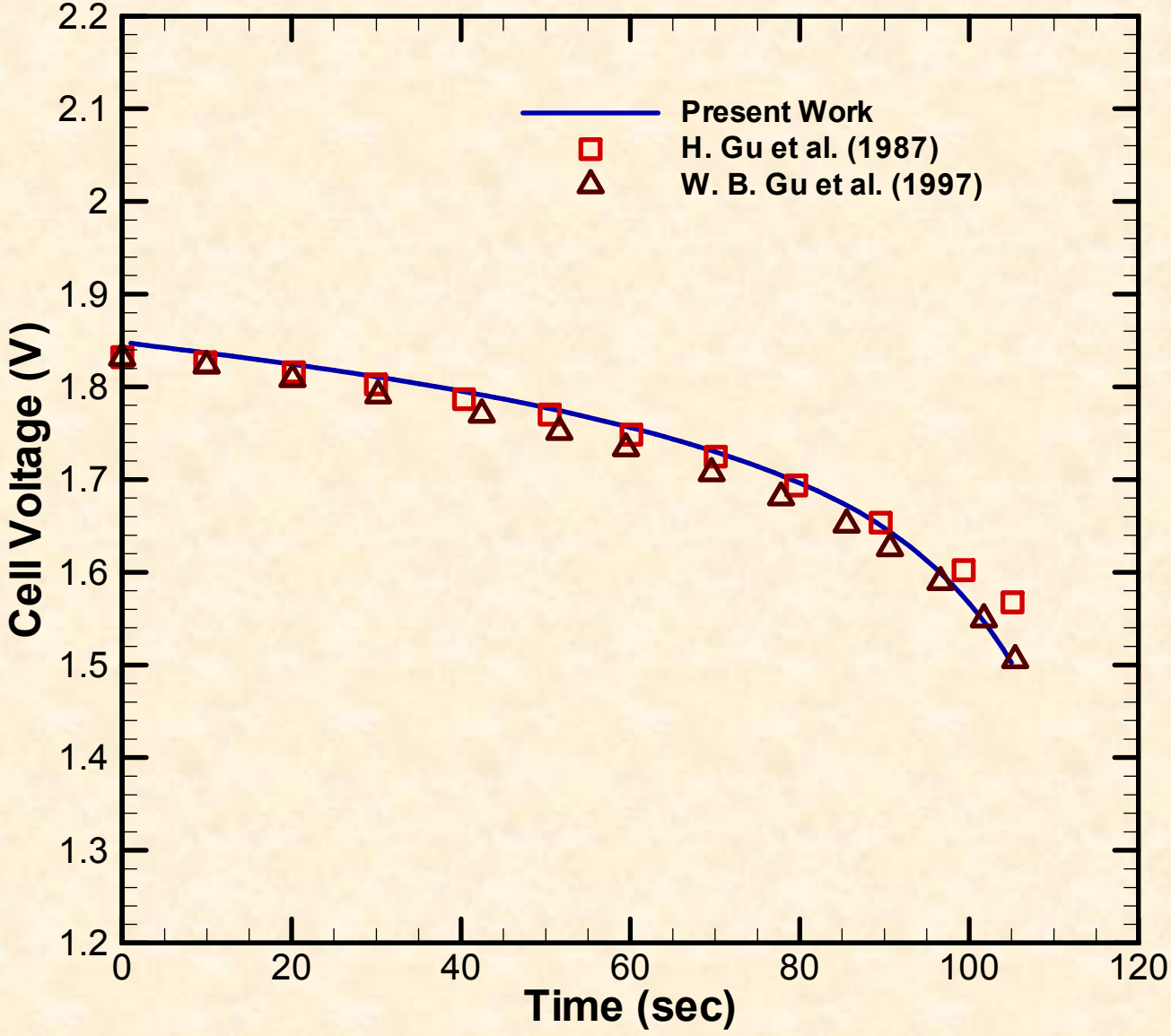
Simulated Acid Concentration



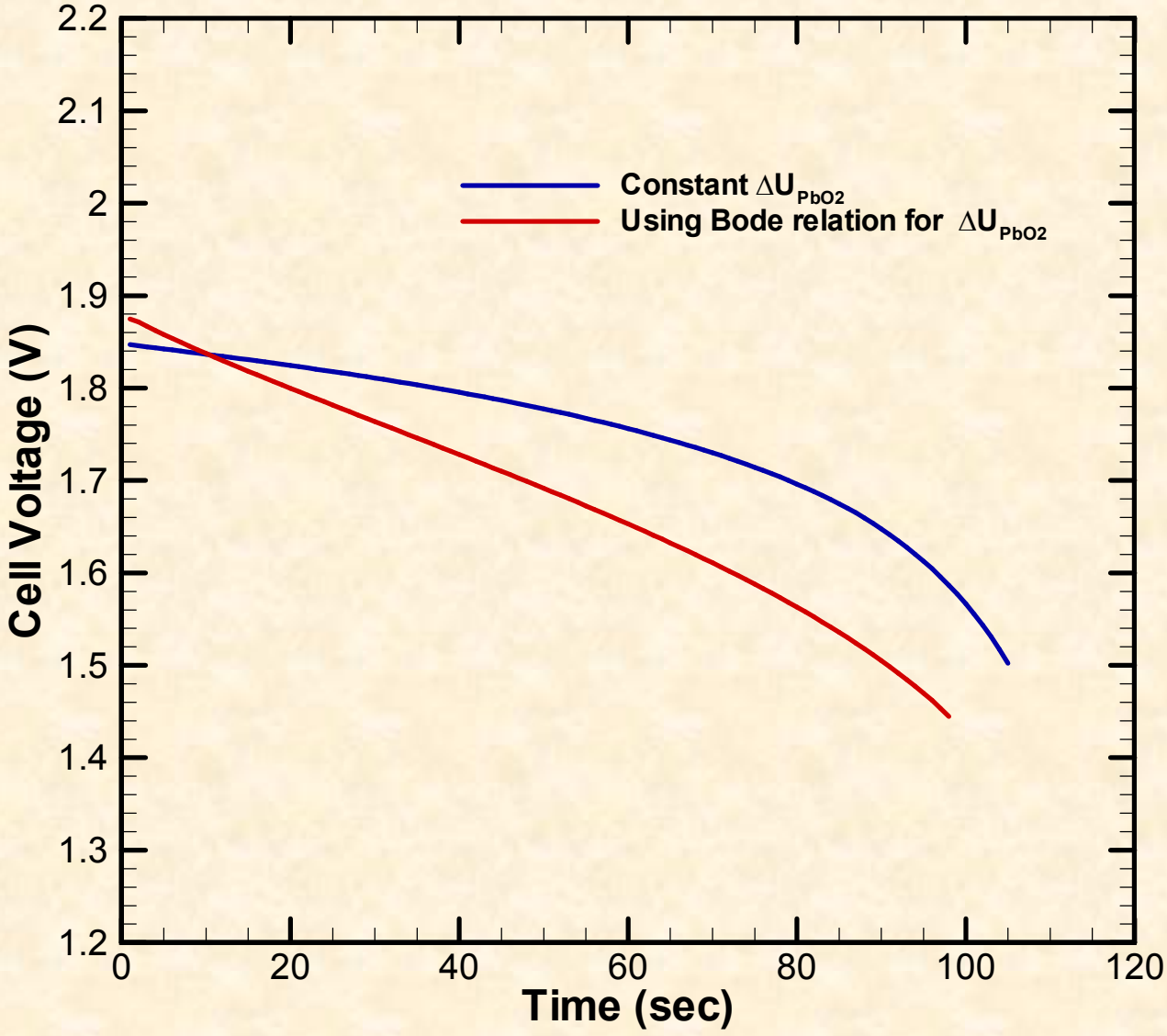
Charge in Battery



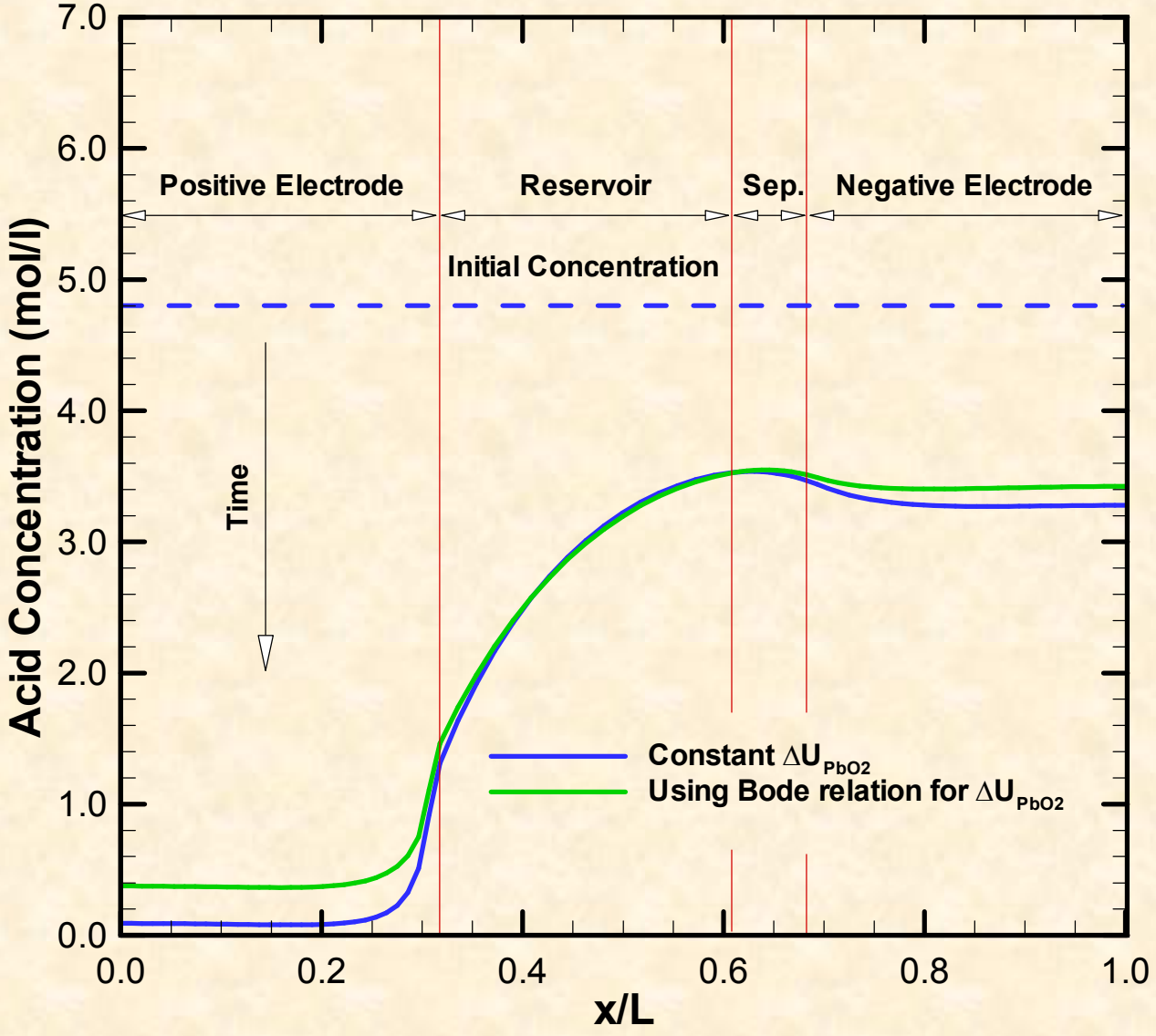
Simulated Cell Voltage



Effect of over potential on cell voltage



Effect of over potential (Acid Concentration)



Conclusions

- Transport equations of battery are solved using Keller-Box method
- The results show good agreement with previous calculations
- This model can be used for simulation and design of batteries
  - The model costs less compared to experiment
  - Modeling is much faster than experiment

Future works

- Simulating more complicated models including other phenomena
  - Oxygen evolution in VRLA
  - Coupling energy equation for investigating the effect of temperature on battery behavior
- Simulation of two-dimensional model
- Obtaining necessary parameters for dynamic modeling

Thanks