LECTURE 06

# Basic Functions of COMSOL Multiphysics

Department of Analytical, Colloidal Chemistry and Technology of Rare Elements

Modeling of chemico-technological processes | 6B07102 Chemical Engineering

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# Purpose and expected learning outcomes

Purpose: move from the hand-written code of Lecture 05 to a finite-element model in COMSOL, and keep the same standards of verification.

### NAVIGATE

The Model Builder tree: definitions, geometry, materials, physics, mesh, study, results.

### PARAMETRIZE

A model with units, global parameters and variables that can be swept.

### SELECT

Primary, secondary or tertiary current distribution from the Wagner number.

### MESH

Boundary layers and graded meshes where concentration gradients are steep.

### SOLVE

Stationary, parametric and time-dependent studies with controlled time steps.

### EVALUATE

Currents, charges and thickness maps by integration, and test mesh independence.

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# The COMSOL workflow in six steps

### 01 Parameters
Global definitions with units

### 02 Geometry
Domains and named boundary selections

### 03 Physics
Interfaces, boundary and initial values

### 04 Mesh
Size, distribution, boundary layers

### 05 Study
Stationary, time-dependent, sweeps

### 06 Results
Plots, derived values, export

**Running example: copper deposition from 0.10 M $CuSO_4$ + 1 M $H_2SO_4$, solved in 1D (transport) and 2D (current distribution)**

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# Model Builder: one tree, one model

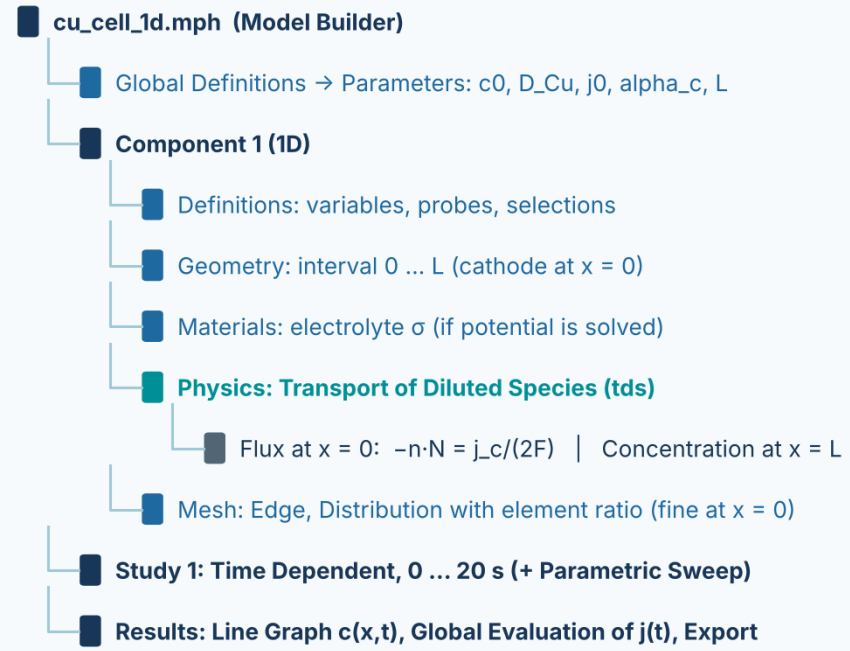
Every node in the tree is one modelling decision; the tree is read top to bottom.

**Parameters → Geometry → Physics → Mesh → Study → Results**

**MODEL CONDITIONS** Global Definitions hold parameters for all components; each Component has its own geometry, physics and mesh. A model can contain several studies.

**EXAMPLE** The 1D Cu model of Lecture 05 rebuilt in COMSOL: one Transport of Diluted Species interface, a flux condition at the cathode and a fixed concentration at x = L.

**EXAMPLE · MODEL TREE OF cu_cell_1d.mph**




**ENGINEERING INTERPRETATION** Name nodes and selections clearly; a reviewer should understand the model from the tree alone.

Further reading: COMSOL Multiphysics Reference Manual and Electrochemistry Module User's Guide (v6.x); Dickinson, Ekström & Fontes, Electrochem. Commun. 40 (2014) 71–74.

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# Parameters, variables and units

Enter every quantity with its unit; COMSOL converts to SI and checks consistency.

| Name | Expression | Description |
|---|---|---|
| c0 | 0.1[mol/L] | bulk $Cu^{2+}$ concentration |
| D_Cu | 7.2e-10[m^2/s] | $Cu^{2+}$ diffusion coefficient |
| j0 | 10[A/m^2] | exchange current density (assumed) |
| alpha_c | 0.5 | cathodic transfer coefficient |
| kappa | 50[S/m] | electrolyte conductivity |
| L | 0.5[mm] | length of the 1D domain |
| eta_app | -0.3[V] | applied overpotential (swept) |
| T0 | 298.15[K] | temperature |

## VARIABLES AND CONSTANTS

**Constants** use built-in F_const and R_const instead of typing numbers.

**Variables** f = F_const/(R_const*T0); j_lim = 2*F_const*D_Cu*c0/delta.

**Unit check** 0.1[mol/L] is stored as 100 $mol/m^3$; an inconsistent sum ($A/m^2$ + V) raises a unit warning.

**Sweeps** any parameter (c0, eta_app) can be varied by a Parametric Sweep.

**ENGINEERING INTERPRETATION** Parameters define the inputs; variables collect derived expressions that are reused in physics and results.

Further reading: COMSOL Multiphysics Reference Manual and Electrochemistry Module User's Guide (v6.x); Dickinson, Ekström & Fontes, Electrochem. Commun. 40 (2014) 71–74.

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# Choosing the physics interface

Primary, secondary and tertiary current distributions differ in what limits the current.

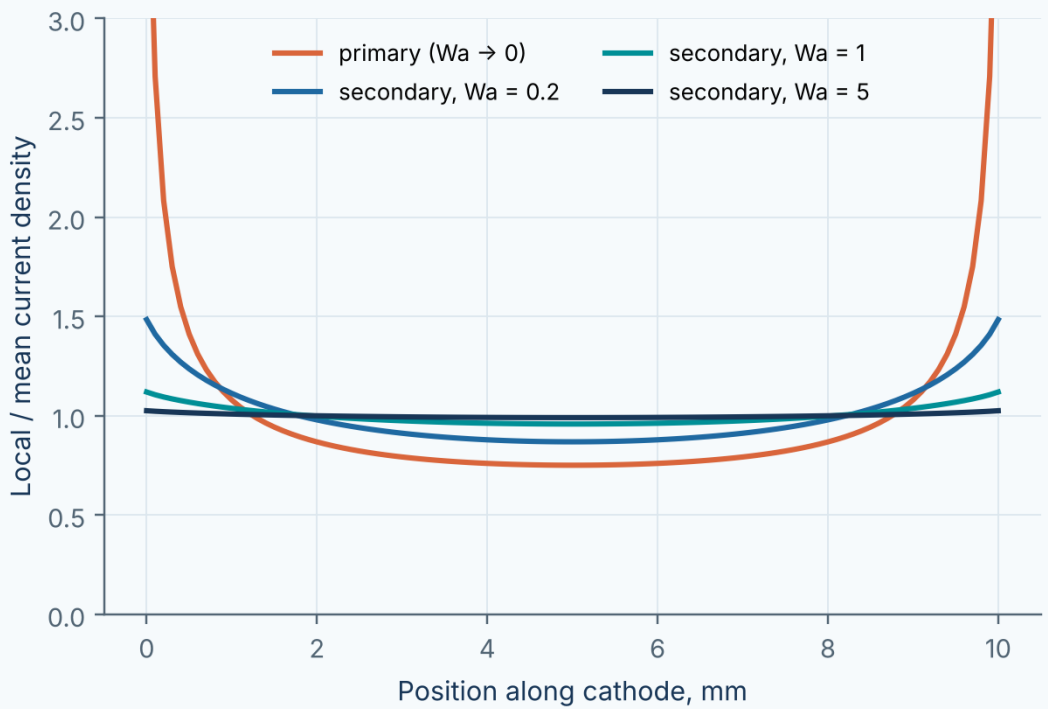
$$Wa = \kappa (\partial\eta/\partial j) / L$$

$$\text{Tafel: } \partial\eta/\partial j = RT / (\alpha_c F|j|)$$

**MODEL CONDITIONS** Primary: ohmic only, ϕ fixed at electrodes. Secondary: adds electrode kinetics. Tertiary (Nernst–Planck): adds concentration variation.

**EXAMPLE** $\kappa = 50\ S\ m^{-1}$, $\alpha_c = 0.5$, $|j| = 200\ A\ m^{-2}$, $L = 1$ cm gives $Wa \approx 1.3$: the local current stays within about 10 % of the mean. For a 10 cm plate $Wa \approx 0.13$ and edges dominate.

EXAMPLE · 2D CELL, CURRENT ALONG A 10 mm CATHODE




**ENGINEERING INTERPRETATION** Small Wa (large parts, fast kinetics) means strong edge build-up; add kinetics before using a primary model.

Further reading: Newman & Balsara, Electrochemical Systems, 4th ed. (2021), ch. 18–19 (current distribution); COMSOL Electrodeposition Module User's Guide (v6.x).

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# Geometry and boundary selections

Boundary conditions are assigned to named selections, not to coordinates.

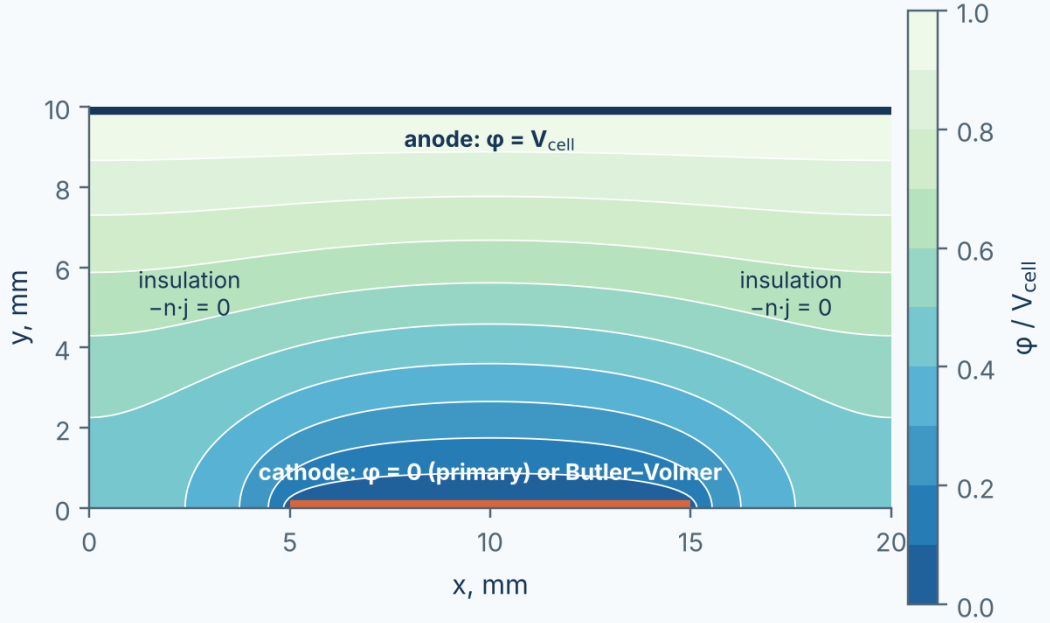
$$-n \cdot j = 0 \quad \text{(insulation)}$$

$$\phi_s - \phi_l - E_{eq} = \eta \quad \text{(electrode)}$$

**MODEL CONDITIONS** 2D cell 20 × 10 mm: cathode is the 10 mm centre part of the lower wall, anode the full upper wall, all other walls insulating.

**EXAMPLE** Primary distribution: equipotential lines crowd near the cathode ends, where the field and the current density are highest.

EXAMPLE · POTENTIAL FIELD, PRIMARY DISTRIBUTION




**ENGINEERING INTERPRETATION** Split the geometry so cathode, anode and walls are separate boundaries; reuse named selections.

Further reading: Newman & Balsara, Electrochemical Systems, 4th ed. (2021), ch. 18–19 (current distribution); COMSOL Electrodeposition Module User's Guide (v6.x).

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# Mesh: resolving boundary layers

Element size must follow the steepest gradient, not the size of the domain.

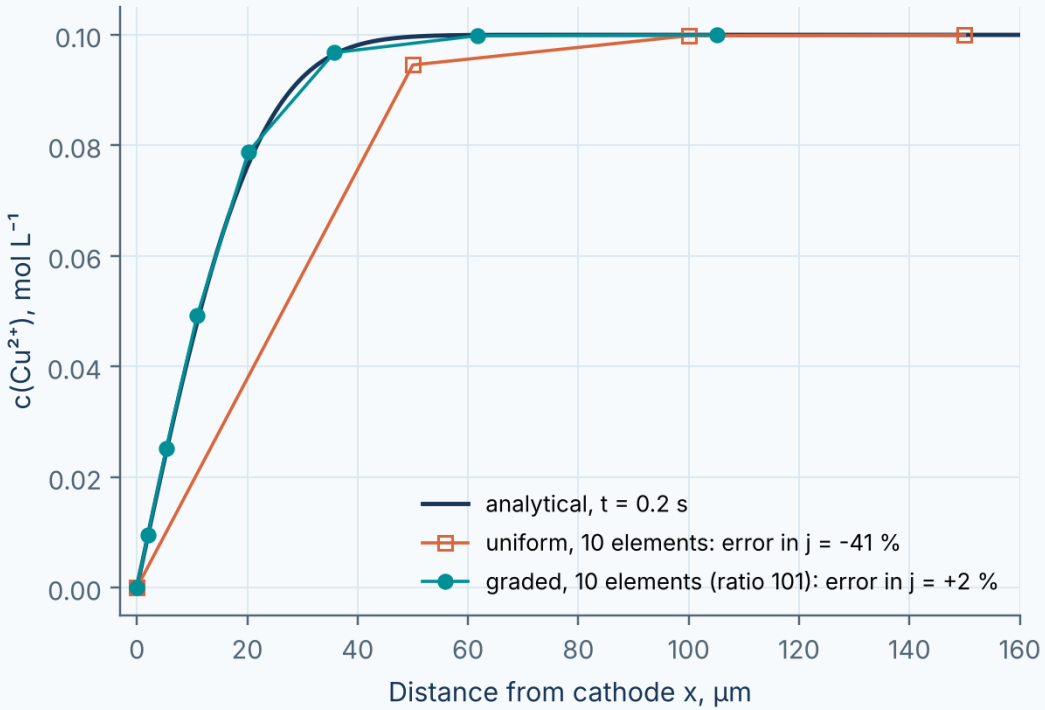
$$\delta(t) \approx (\pi D t)^{1/2}$$

$$\text{element ratio} = h_{max} / h_{min}$$

**MODEL CONDITIONS** 1D domain 500 µm, potential step, t = 0.2 s (δ ≈ 21 µm). Edge mesh with a Distribution node; element ratio 101 gives $h_{min}$ = 2 µm.

**EXAMPLE** Error in current: uniform 10 elements −41 %; graded 10 elements +2.2 %; uniform 100 elements +3.1 %. Ten graded elements beat one hundred uniform ones.

**EXAMPLE · SAME NUMBER OF ELEMENTS, DIFFERENT ACCURACY**




**ENGINEERING INTERPRETATION** In 2D, add Boundary Layers at electrodes and report results on at least two meshes (mesh independence).

Further reading: COMSOL Multiphysics Reference Manual and Electrochemistry Module User's Guide (v6.x); Dickinson, Ekström & Fontes, Electrochem. Commun. 40 (2014) 71–74.

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# Stationary study with a parametric sweep

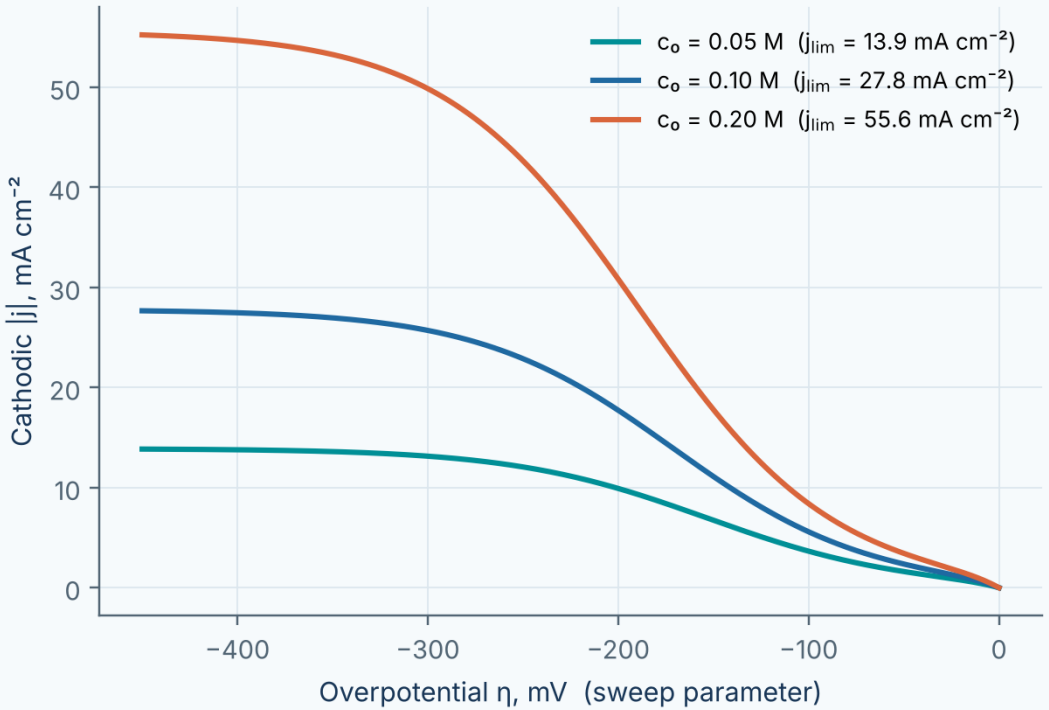
A stationary study solves for steady state; a sweep repeats it for a list of values.

**$F(u, p) = 0$, $p = \eta_{app}, c_0, \ldots$**
**range(-0.45, 0.01, 0) [V]**

**MODEL CONDITIONS** Butler–Volmer at the cathode, Nernst layer δ = 50 µm; $j_0$ scaled as $c_0^{0.5}$. Strongly nonlinear kinetics converge best when η is stepped from 0.

**EXAMPLE** Sweeping η for $c_0$ = 0.05, 0.10 and 0.20 M gives plateaus of 13.9, 27.8 and 55.6 mA cm$^{-2}$; $j_{lim}$ is proportional to $c_0$.

**EXAMPLE · POLARIZATION CURVES FROM A PARAMETRIC SWEEP**




**ENGINEERING INTERPRETATION** Use an Auxiliary sweep (continuation) when the solver fails: each solution is the start value for the next.

Further reading: COMSOL Multiphysics Reference Manual and Electrochemistry Module User's Guide (v6.x); Dickinson, Ekström & Fontes, Electrochem. Commun. 40 (2014) 71–74.

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# Time-dependent study and solver settings

Implicit BDF time stepping is stable; accuracy is set by tolerances and output times.

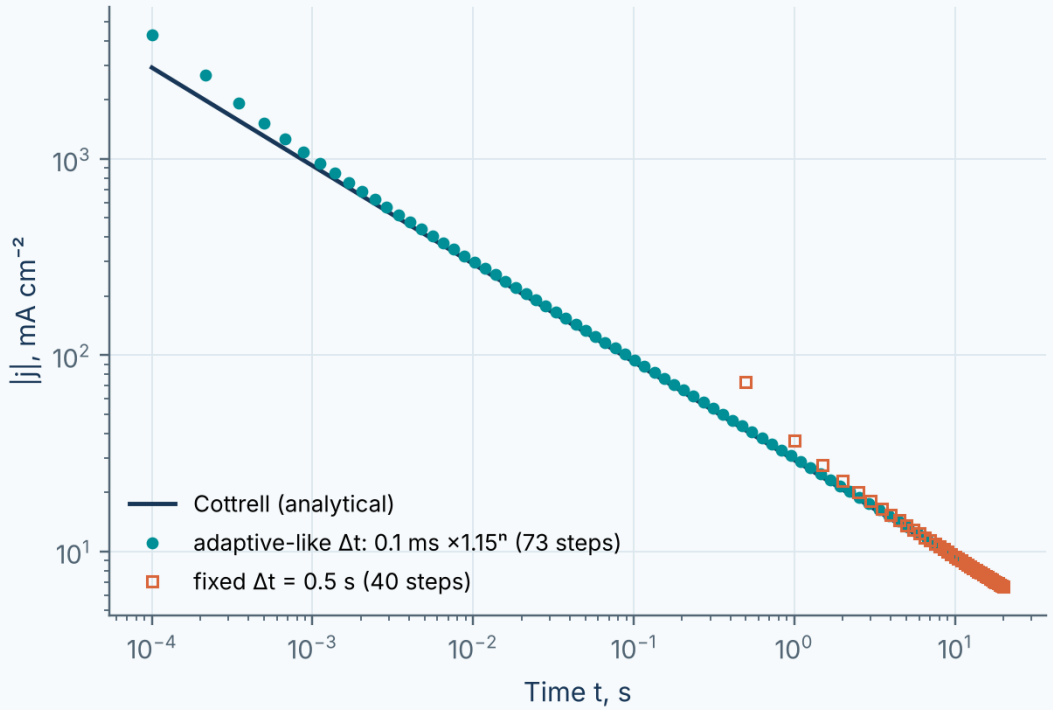
**M du/dt + K u = f,  BDF**

**Output times ≠ solver time steps**

**MODEL CONDITIONS** Potential step at t = 0 creates a singular current ($j \propto t^{-1/2}$); the first steps must be very small. Free steps let the solver adapt.

**EXAMPLE** Steps growing from 0.1 ms by ×1.15 (73 steps) follow Cottrell after the first few steps (2.8 % at 20 s). Fixed Δt = 0.5 s misses all early data and is 25 % wrong at t = 1 s.

**EXAMPLE · CHRONOAMPEROMETRY, IMPLICIT TIME STEPPING**




**ENGINEERING INTERPRETATION** Ramp step changes over a short time (e.g. a smoothed step function) to avoid inconsistent initial values.

Further reading: COMSOL Multiphysics Reference Manual and Electrochemistry Module User's Guide (v6.x); Dickinson, Ekström & Fontes, Electrochem. Commun. 40 (2014) 71–74.

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# Post-processing: derived values and maps

Integrate local results to obtain quantities that can be measured.

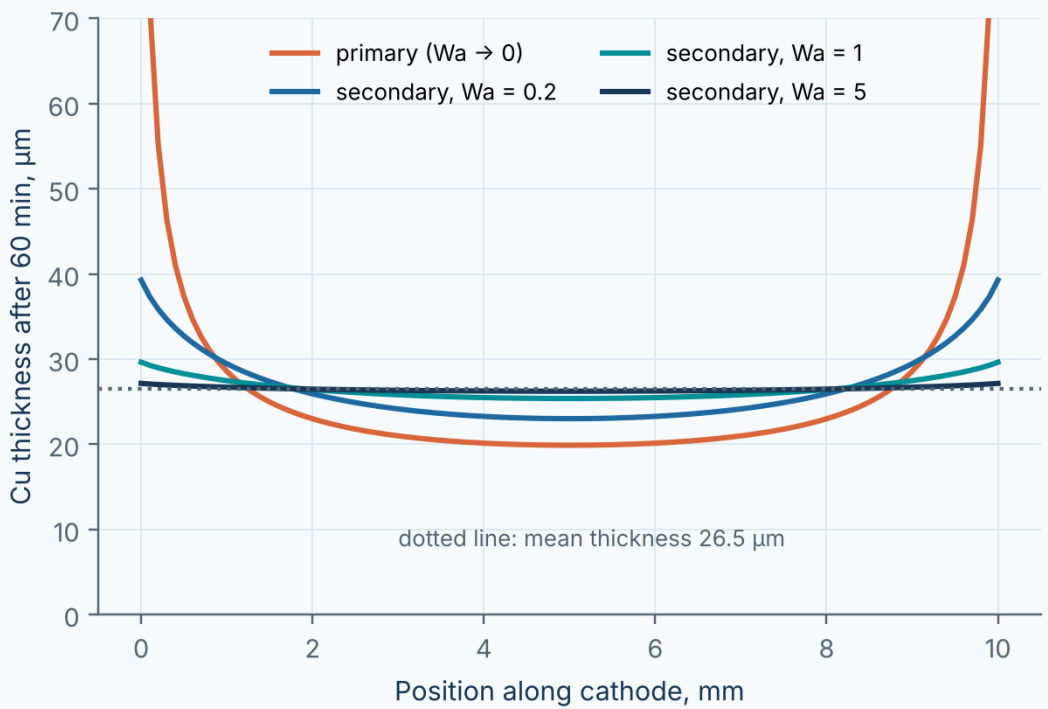
$$I = \int_A j \cdot n \, dA, \quad Q = \int I \, dt$$

$$h = M \, Q_{local} / (nF\rho)$$

**MODEL CONDITIONS** 2D cell from slide 7, mean current density 200 A $m^{-2}$, 60 min, 100 % current efficiency; local thickness from local charge.

**EXAMPLE** Mean thickness 26.5 µm. With Wa = 1 it ranges 25.4–29.6 µm; with Wa = 0.2, 23.0–39.3 µm; the primary model predicts unbounded edge growth.

**EXAMPLE · DEPOSIT THICKNESS AFTER 60 min**




**ENGINEERING INTERPRETATION** Use Line/Surface Integration and Global Evaluation; export tables with units for comparison with profilometry.

Further reading: Newman & Balsara, Electrochemical Systems, 4th ed. (2021), ch. 18–19 (current distribution); COMSOL Electrodeposition Module User's Guide (v6.x).

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# Common errors and how to detect them

## UNITS

Missing brackets: 0.1 without [mol/L] is read as 0.1 mol/$m^3$. Check the unit column in Parameters.

## SIGNS

Inward vs outward normal flux. Check that the integrated $Cu^{2+}$ flux equals I/(nF).

## INITIAL VALUES

Inconsistent start ($c = c_0$ while $c(0) = 0$) – smooth the step or start from a stationary solution.

## MESH

No refinement at electrode edges. Compare results on two meshes; differences must be small.

## SOLVER

Divergence at high η. Use continuation (auxiliary sweep) and good start values.

## REPORTING

No record of settings. Save the .mph, list parameters, mesh statistics and tolerances.

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# Conclusions: a verified model is a useful model

### STRUCTURE

The Model Builder tree documents the model; name nodes and selections.

### PARAMETERS

Units in brackets and built-in constants prevent most input errors.

### PHYSICS

Choose the current distribution by the Wagner number, not by habit.

### MESH

Graded and boundary-layer meshes resolve thin diffusion layers cheaply.

### STUDIES

Sweeps and continuation for nonlinear steady states; small first steps for transients.

### RESULTS

Integrated currents, charges and thicknesses link the model to experiment.

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# Homework: calculations, interpretation and research

**1. THEORY** Compare the primary, secondary and tertiary current distribution interfaces: which variables are solved and which boundary conditions are needed at the cathode?

**2. CALCULATION** Find the Wagner number for $\kappa = 30\ \mathrm{S\ m^{-1}}$, $\alpha_c = 0.5$, $|j| = 150\ \mathrm{A\ m^{-2}}$ and plate lengths of 5 mm and 50 mm. Which plate needs a secondary model?

**3. MODEL** Build the 1D chronoamperometry model in COMSOL (Transport of Diluted Species). Compare the current at 0.1, 1 and 10 s with the Cottrell equation on two meshes.

**4. CRITIQUE** Run the model with a uniform mesh of 10 elements and fixed $\Delta t = 0.5$ s. Explain each deviation using $\delta = (\pi D t)^{1/2}$.

**5. RESEARCH** Open a COMSOL Application Library electrodeposition example and draw its model tree. Identify every assumption and one quantity you could measure to validate it.

Constants: $F = 96485\ \mathrm{C\ mol^{-1}}$; $R = 8.314\ \mathrm{J\ mol^{-1}\ K^{-1}}$; $T = 298.15$ K; $D(Cu^{2+}) = 7.2 \cdot 10^{-10}\ \mathrm{m^2\ s^{-1}}$.

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**Recommended Literature**


1. Fogler, H. S. *Elements of Chemical Reaction Engineering*. 5th ed., Pearson, 2016.
2. Himmelblau, D. M., Riggs, J. B. *Basic Principles and Calculations in Chemical Engineering*. 8th ed., Pearson, 2012.
3. Bird, R. B., Stewart, W. E., Lightfoot, E. N. *Transport Phenomena*. 2nd ed., John Wiley & Sons, 2002.
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5. Bequette, B. W. *Process Control: Modeling, Design, and Simulation*. Prentice Hall, 2003.