Simulation of drying process during fabrication of Lithium-Ion Battery porous electrode

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Introduction

Lithium Ion Battery Electrode Manufacturing Process

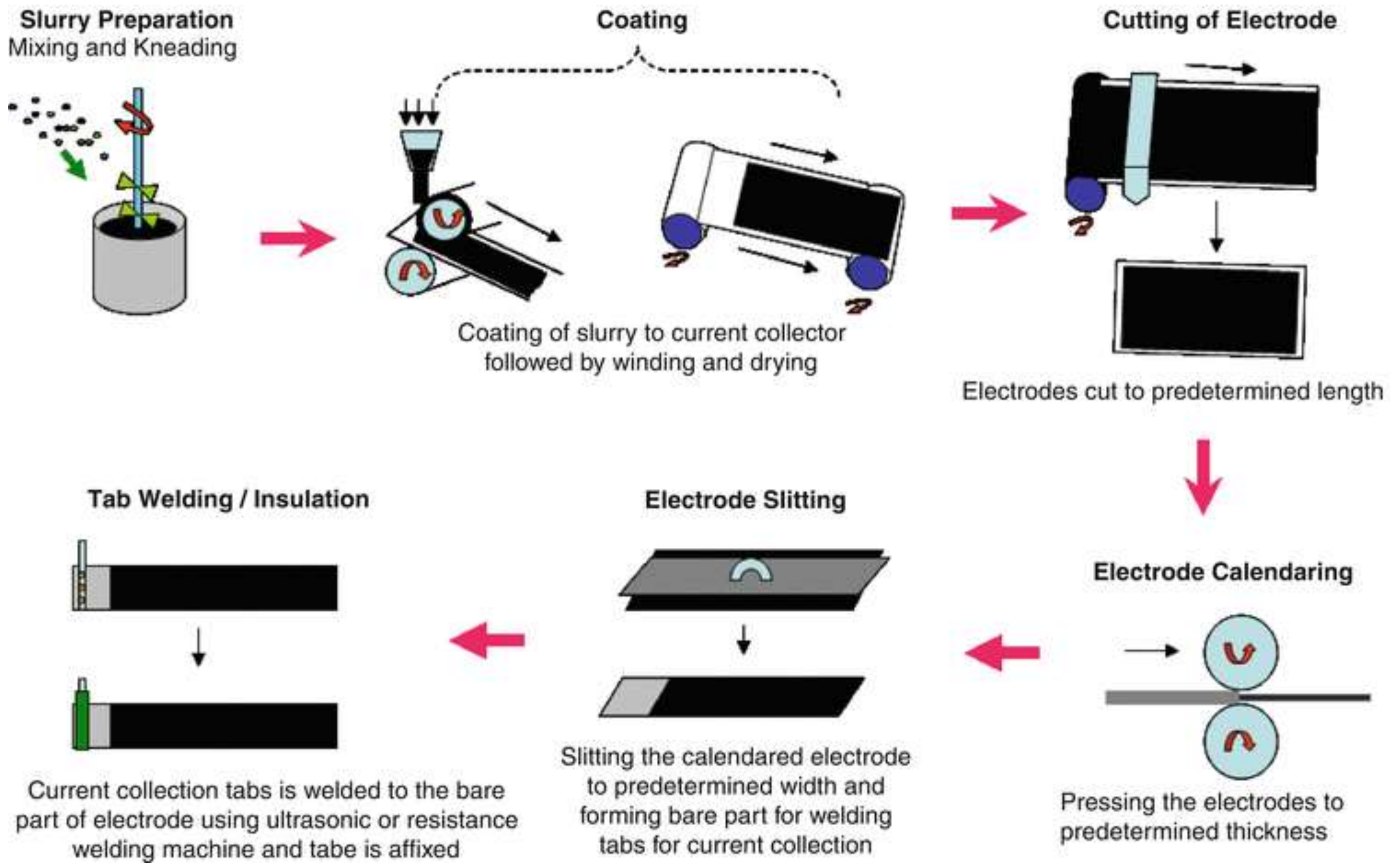
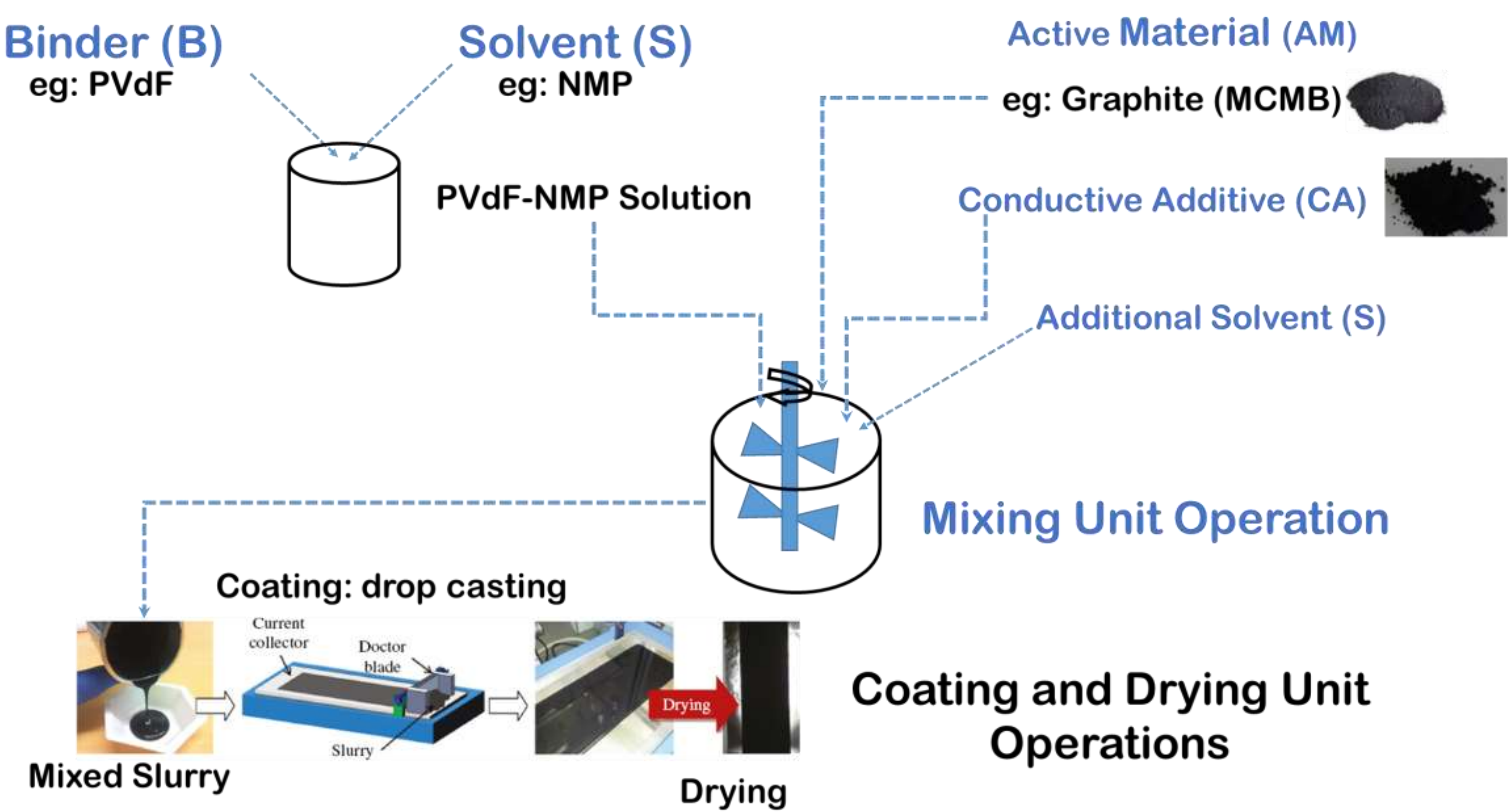
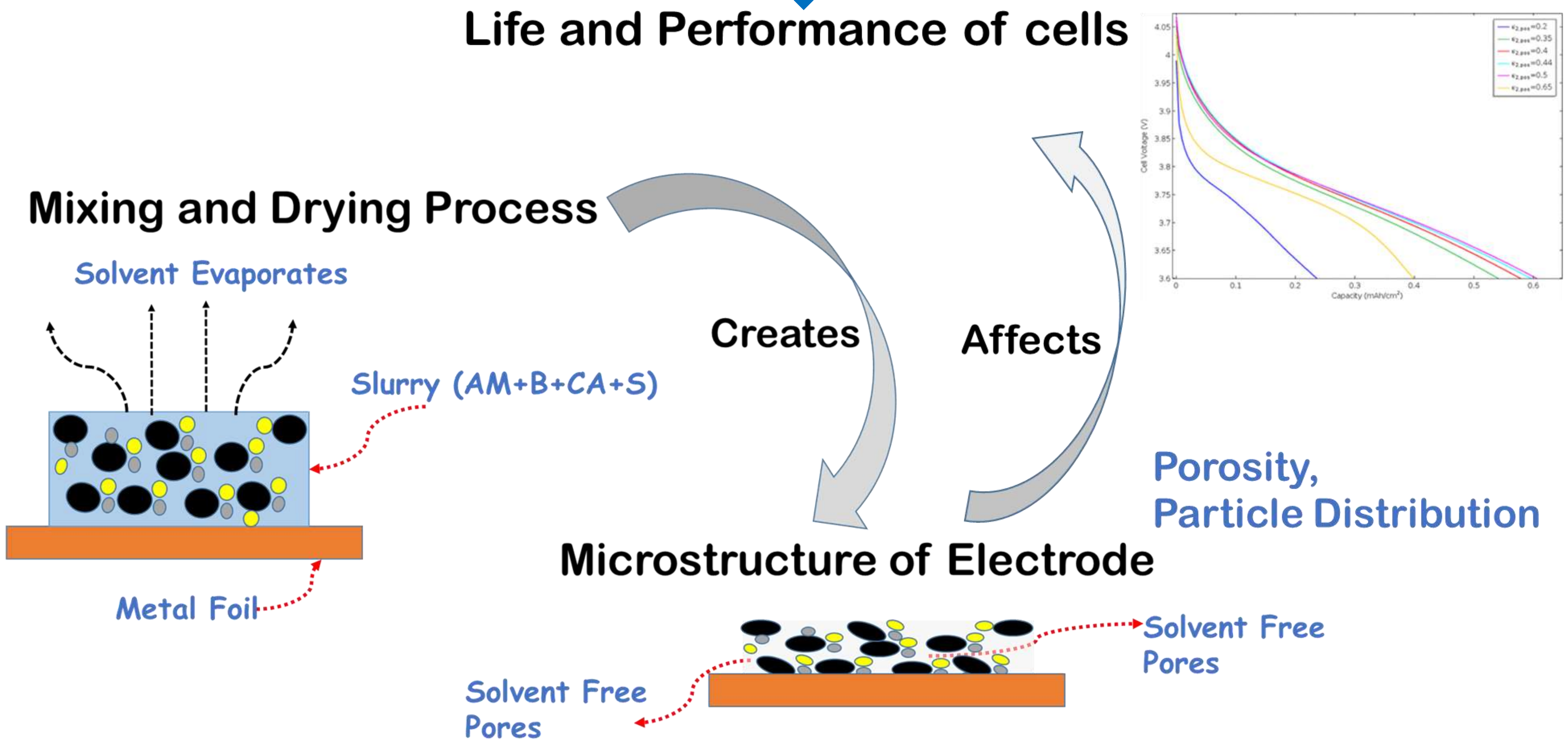


Image Adapted from : *Zhang Z.., Ramadass P. (2012) Lithium-Ion Battery Systems and Technology. In: Meyers R.A. (eds) Encyclopedia of Sustainability Science and Technology. Springer, New York, NY*

Mixing and Coating Unit Operations



Motivation

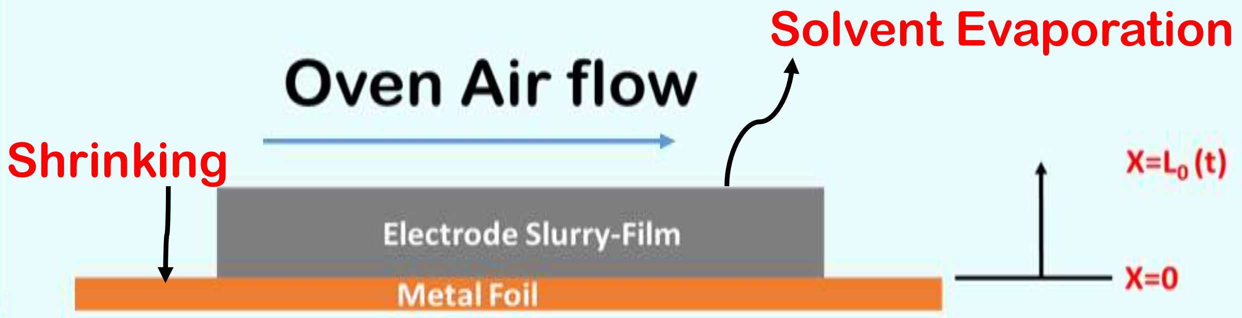


Optimize Battery Electrode Manufacturing Process

Drying Phenomena

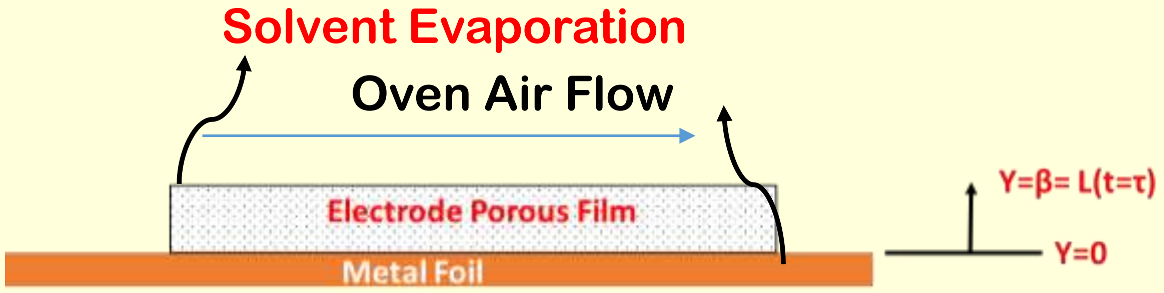
Drying happens in two Stages/Phases

Phase 1- The coating dries at almost constant rate where solid consolidation **(Shrinking of coating)** happens and solvent evaporates



Schematics of geometry being considered in Phase 1

Phase 2- Evaporation continues beyond shrinking removing solvent from pores created



Schematics of geometry being considered in Phase 2

Drying Model Development

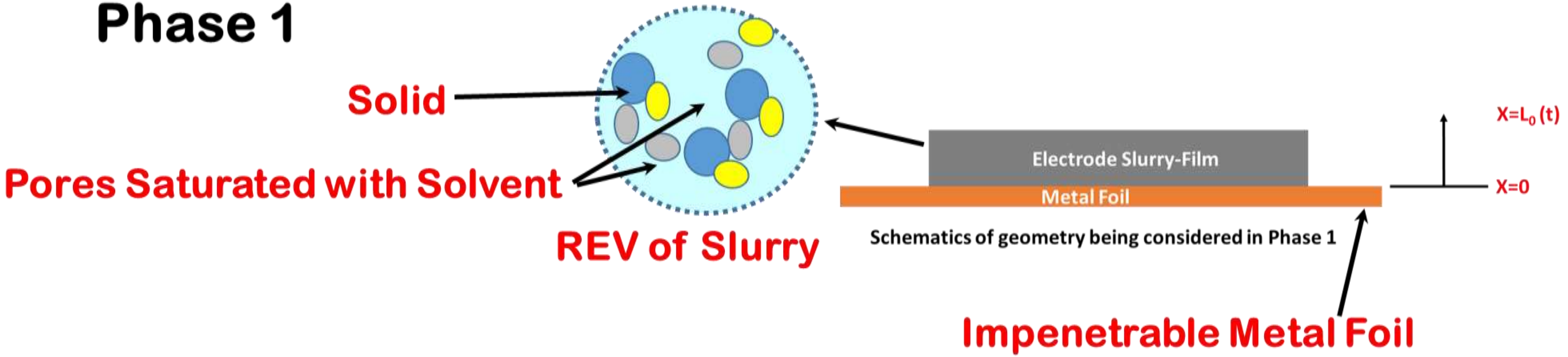
Assumptions

- All solids (AM, B and CA) are treated together as single solid phase (Binder Migration is ignored).
- Shrinking happens only along the thickness direction (Area remains the same).
- Edge effects are ignored and drying along thickness direction is only considered.
- Temperature is constant *(Oven is maintained at isothermal condition and sample size is small).*
- Phase I is treated as saturated with liquid solvent.
- Effect of gravity is ignored.
- Gas phase is treated as a single component with both solvent vapour and dry air.

Drying Model Development

Model Geometry & Transport Phenomena

Phase 1

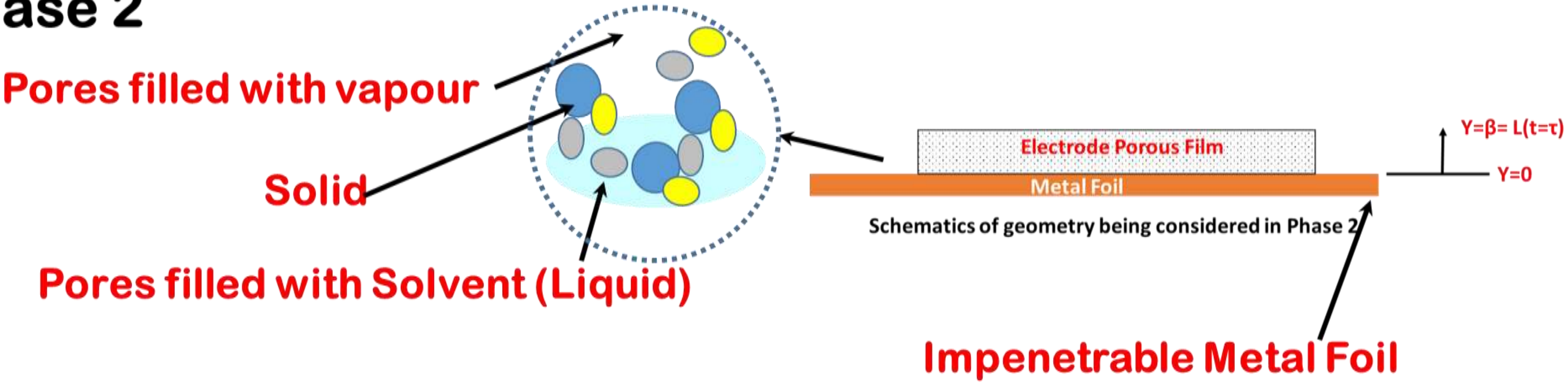


- Mass Conservation of Liquid Solvent in Suspended Solid Medium
- Momentum balance of Liquid Solvent in Suspended Solid Medium
- Movement of Solid or Coating (Shrinking)

Drying Model Development

Model Geometry & Transport Phenomena

Phase 2



- Mass Conservation of Liquid Solvent in Porous Medium
- Mass Conservation of Solvent in Vapour Phase in Porous Medium
- Momentum balance of Solvent in Porous Medium

Governing Equations

Solvent Mass Conservation (liquid phase):

$$\frac{\partial}{\partial t}(\rho_l \varepsilon_l)+\frac{\partial}{\partial t}(\rho_l \varepsilon_l u_l)=0 \quad \textbf{(Phase 1)}$$

$$= -m \quad \textbf{(Phase 2)}$$

Solvent Mass Conservation (Gas phase):

$$\frac{\partial}{\partial t}(\rho_g \varepsilon_g)+\frac{\partial}{\partial t}(\rho_g \varepsilon_g u_g)=m \quad \textbf{(Phase 2)}$$

Solvent Velocity:

$$u_i = \frac{K\kappa_i}{\mu_l \varepsilon_i}\left(\frac{\partial P_i}{\partial x}\right); \; i= l\,,\, g$$

Coating Shrinking:

$$u_s = -\frac{1}{A\rho_l}\frac{dw}{dt} \quad \textbf{(Phase 1)}$$

Approach Using COMSOL

Modules Used

Transport Phenomena	Phase 1	Phase 2
Mass Conservation of liquid Phase:	General PDE	General PDE with Source term
Mass Conservation of Vapour Phase:	----	General PDE with Source term
Velocity of Liquid Phase:	Darcy's Law	Darcy's Law
Velocity of Vapour Phase:	----	Darcy's Law
Velocity of Solid Phase (*Coating thickness):	Moving Mesh	----

Results & Discussion

Case Study: Drying of Anode in Oven at 80 °C

Sample Experimental Parameters for Validation:

Initial set thickness: 154 μm

Area of coating: 23 cm^2

Total Solid content: 44 % of initial coating

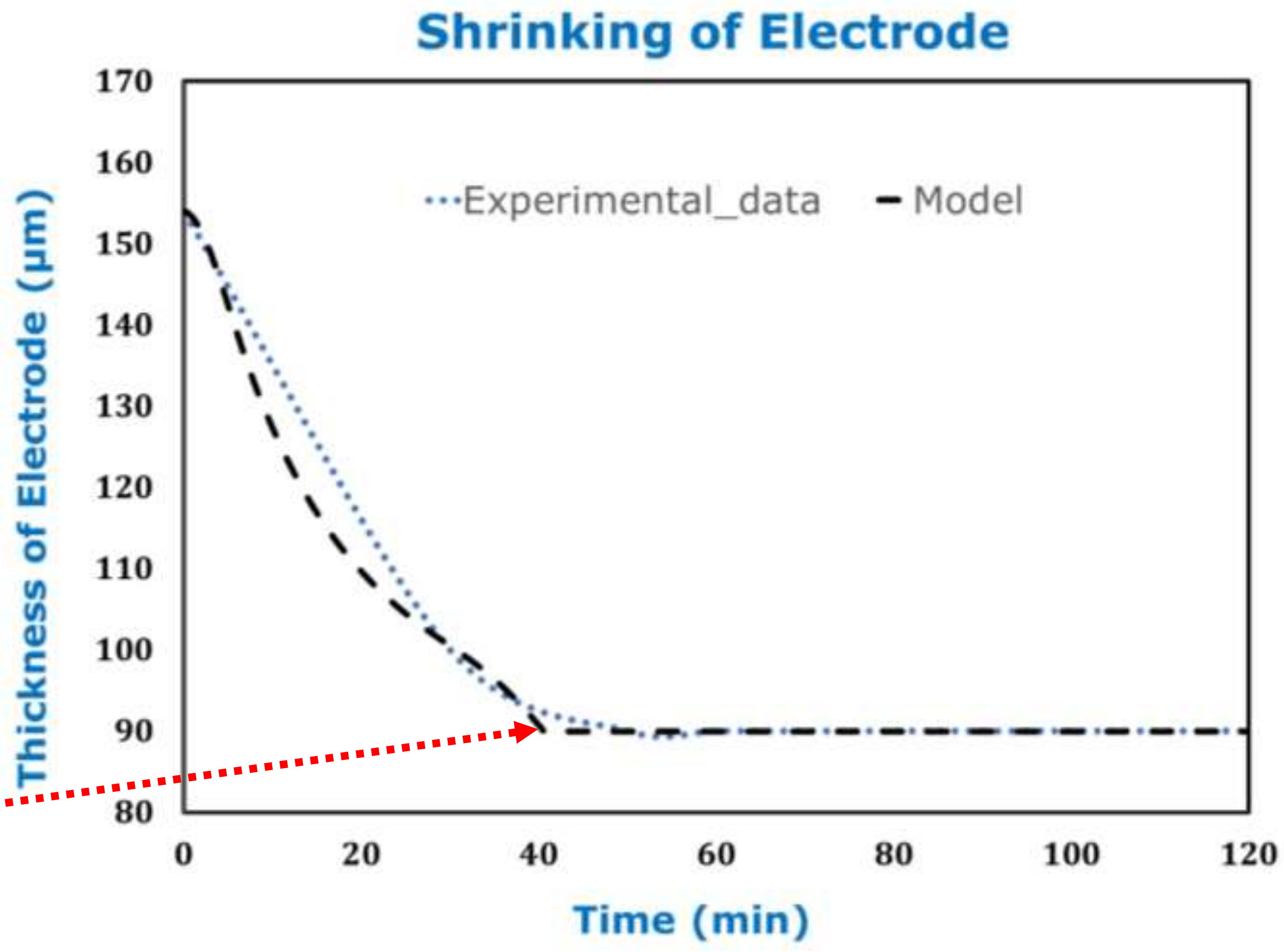
Initial weight of coating: 0.474 g

Final porosity obtained before calendaring: 0.52

Volume fraction of Solvent in the slurry: 0.72

Sample Validation Results

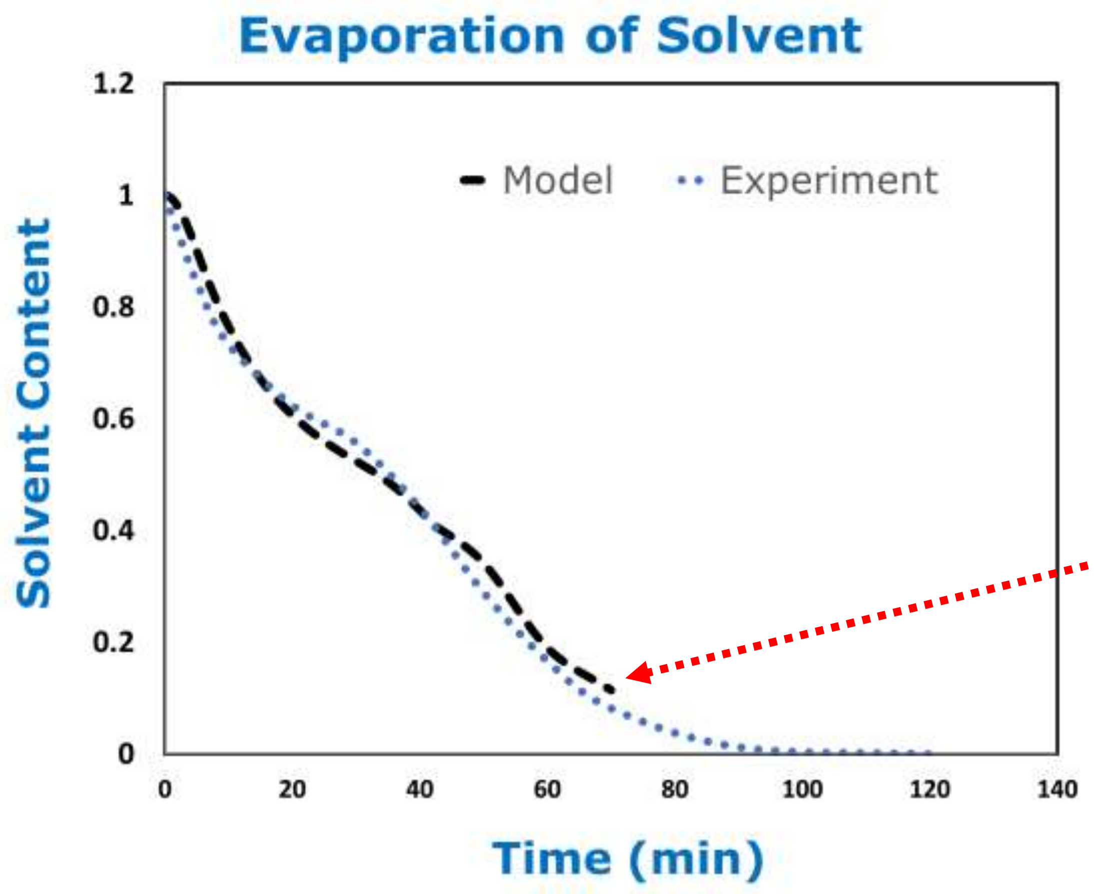
Phase 1(Shrinking of Electrode) Result comparison between model and Experiment



Model Predicts the stopping point of Shrinking accurately

Sample Validation Results

Result comparison between model and Experiment



Phase 2 of the model was stopped at 0.1 saturation

Comparison of Solvent evaporation predicted and measured

Future Extension

- Sedimentation of solid has to be included
- Binder migration has to be included.
- Further refining of estimated mass and heat transfer coefficient from experiments has to be carried out.
- Accurate measurement of thickness is needed for better comparison.
- Parametric studies has to be carried out.

Acknowledgements

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