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Watching Paint Dry: A 2D Model of Latex Film Formation

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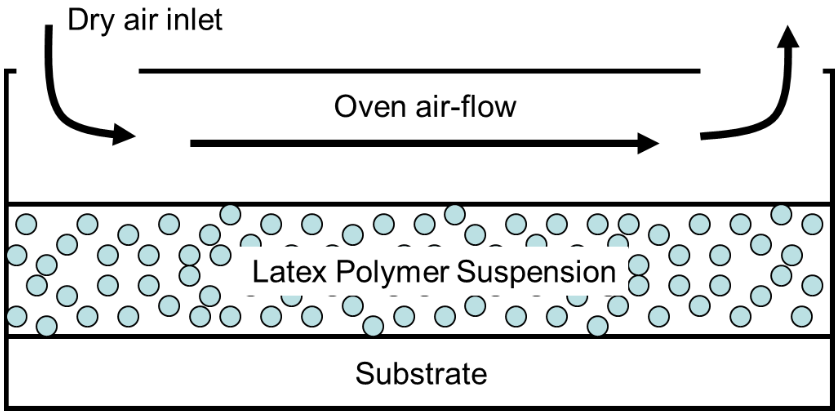
> Introduction

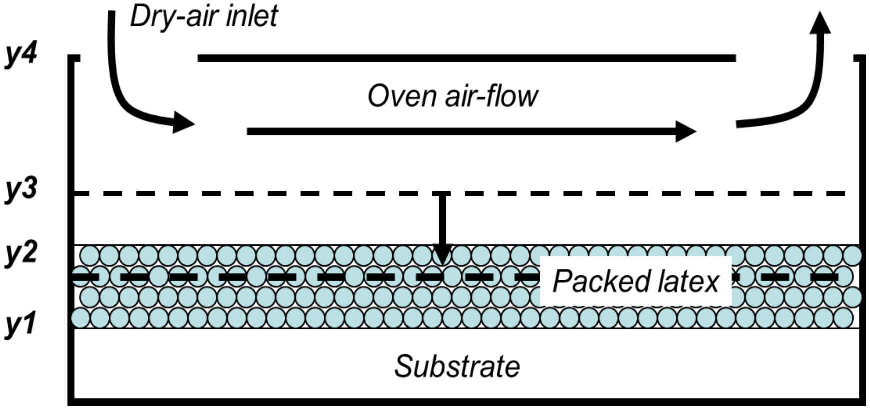
- At ZINK Imaging, we make a coated color-imaging medium, and some layers used latex as a binder
- **Latex is a general name for a suspension of a water-insoluble polymer**, commonly used as a binder for paint and other water-based coatings.
- As the suspension dries, the polymer particles become packed into an array, and if it is above the MFFT (minimum film forming temperature) the polymer particles will coalesce..
- If the particles coalesce before the water is removed, the coating can become permanently tacky
- Question: What is the best drying schedule for smooth layers but highest possible speed?

> Introduction

Stage 1 – The wet coating begins drying at a rate similar to pure water

Stage 2 -- When sufficient water is removed, the particles touch, and form a porous matrix. The air/water matrix then recedes into this matrix





Stage 3 --- The polymer particles coalesce to form a smooth film.

> Multiphysics

- **Problem requires:**
  - **Thermal Model:** Oven air warms the water, but is cooled by evaporation at air/water interface
  - **Fluid dynamics:** Air flow adapts to changing interface shape and carries away water vapor
  - **Dilute species transport:** Water vapor escapes by diffusion through packed latex and by diffusion and advection in the air.

> Complications

- Most of the physics occurs at the **air/water interface**, which is a moving boundary. This requires **moving mesh**.
- However, this boundary is initially **above** the latex but ends up **below** it. The topology changes. Three layers become four layers and then three again.

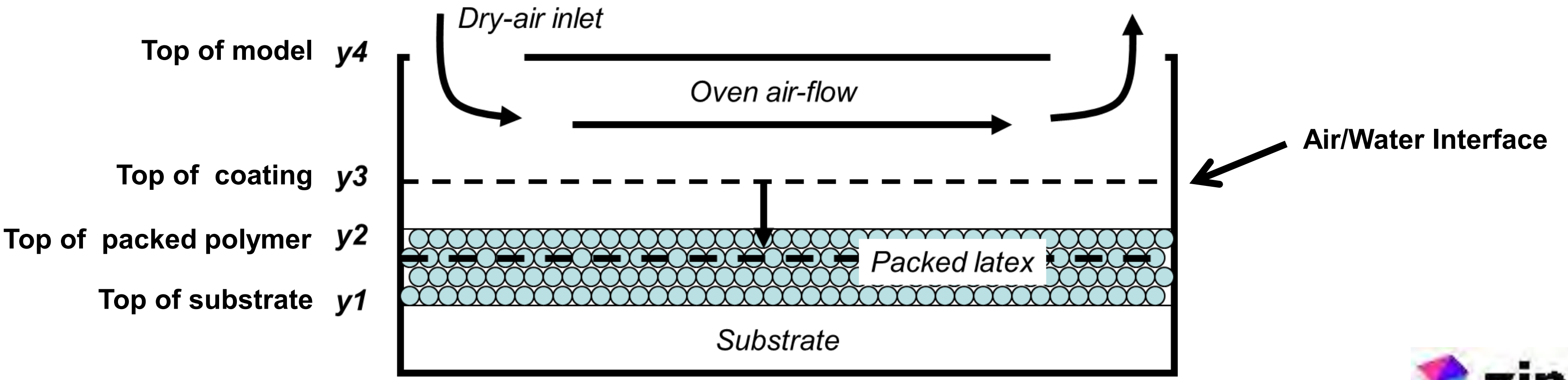
Substrate
Wet latex coating
Oven air

→

Substrate
Wet packed latex
Dry packed latex
Oven air

→

Substrate
Dry packed latex
Oven air



> Approach

- Rather than dealing with these complications, we tried a different method.

- Approach
  - All layers are treated as being porous.
  - Air layer has porosity of 100%.
  - Latex layer has a fill-factor that increases in time until it reaches 74% (close-packed spheres) and then stays constant.
  - Substrate has porosity of 0%.

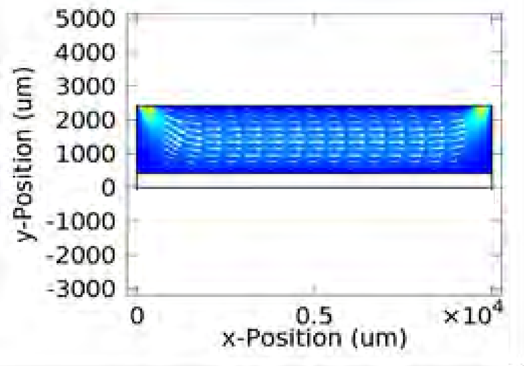
- Porous material has properties that depend on position and time.
  - Example: k=mat1.def.k11*(y >= y1) + mat4.def.k11*(y < y1)
  - Where: k = thermal conductivity, y1 = surface of substrate, mat1 = polymer, mat4 = substrate.

- Moving mesh has a single internal boundary, the air/water interface.

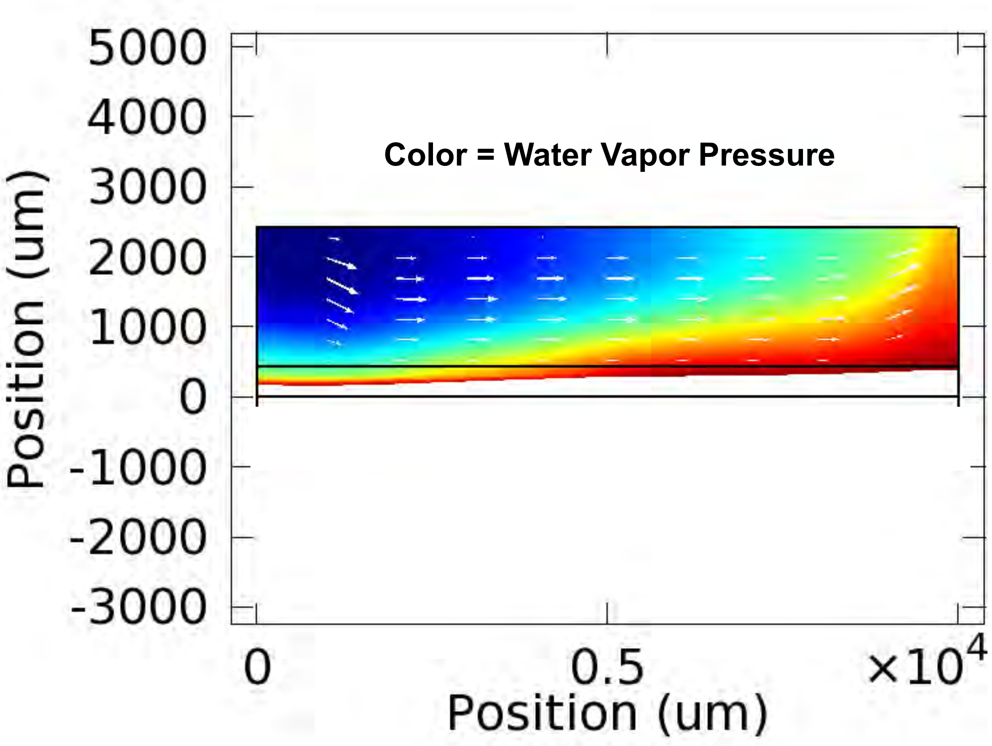
> Assessment

- There are both positive and negative features to this approach.
- **Pros:**
  - The moving mesh issues are highly simplified.
  - The topology problem is removed.
- **Cons:**
  - The geometry does not show the material boundaries, because they are embedded in the expressions for material properties. (Use your imagination!)
  - The expressions for material properties are more complicated (though not as much as you might think).
  - Boundary conditions are potentially trickier.

> Sample Results

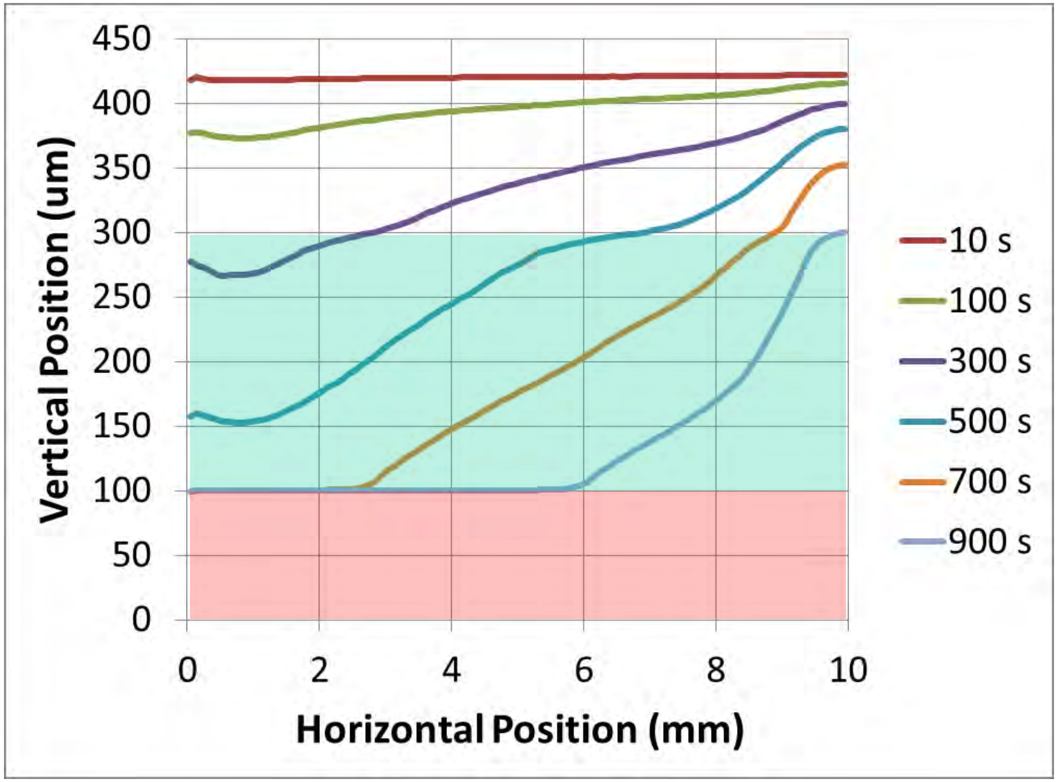


- Dry air enters at the upper left and leaves at the upper right.
- Drying is from left to right, as shown by the profile in the air/water interface.



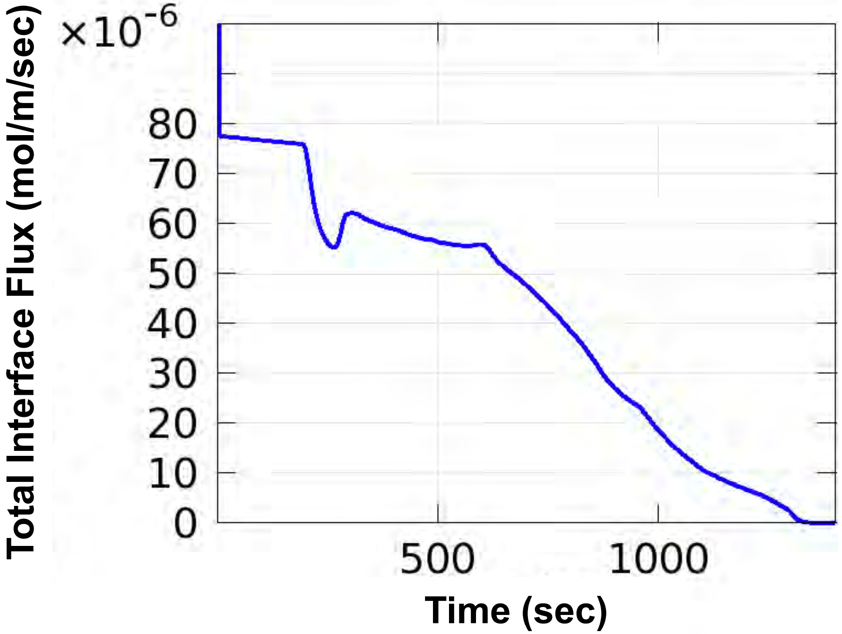
> Air/Water interface profile

- The air/water interface profile can be seen more clearly in this graph.
- The substrate surface is at y=100 um (red area)
- The top of the packed latex is y = 305 um, where several of the graphs show a slight inflection. (blue area)
- In this simulation, T = 295 K and the air velocity is 2 m/sec



> Time Sequence of Drying

- This graph shows the **total flux of water vapor** across the air/water interface as a function of time.
- From t=0 sec to t ~ 200 sec, the water evaporates at a constant rate, like pure water.
- At t~200 sec, the latex is packed at the left hand end, and the air/water interface is entering the pack.
- By t~600 sec, most of the latex is packed, and further evaporation is through the interstices.
- Evaporation continues until t ~ 1400 sec, when the air/water interface reaches the substrate.



T = 295 K
RH = 50%
V_air = 1.8 m/sec

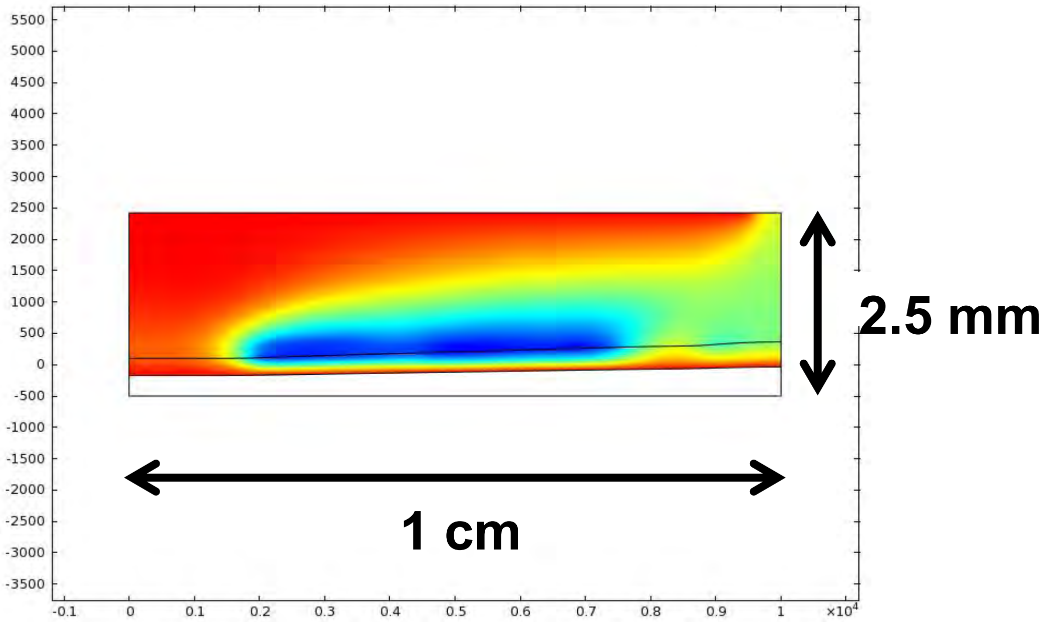
> Temperature profile

- Water evaporation causes the temperature to fall, so a temperature profile reveals where the water is evaporating

- This is a profile at t = 600 sec. for a film that dried in 1200 sec.

- Minimum temperatures (shown in blue) occur in the center of the film, and are working their way towards the right.

- Oven temperature T_oven shows up in red.

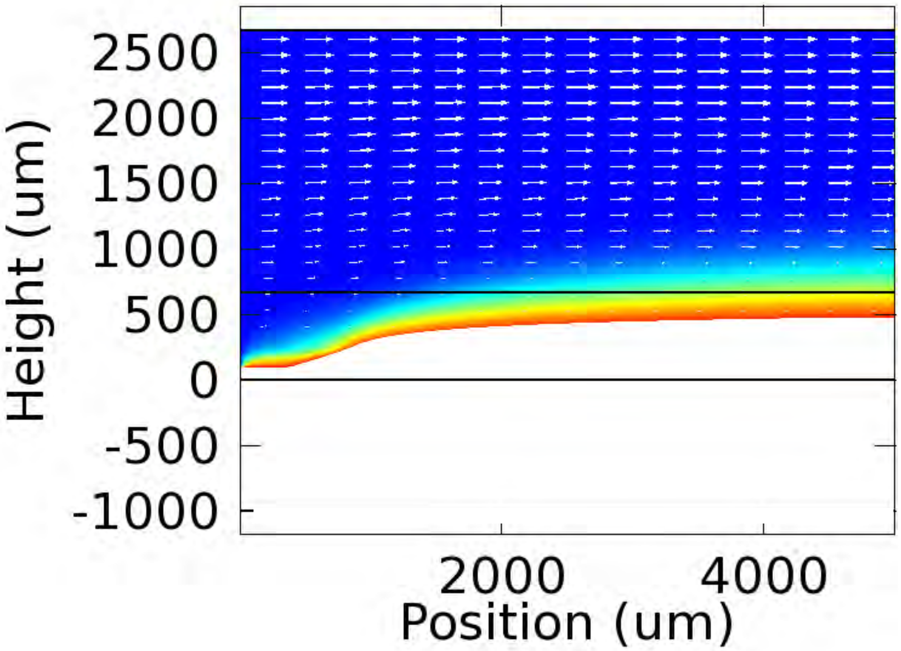


> Drying in laminar air-stream

- We have also made a model in which the air enters on the left and leaves on the right.

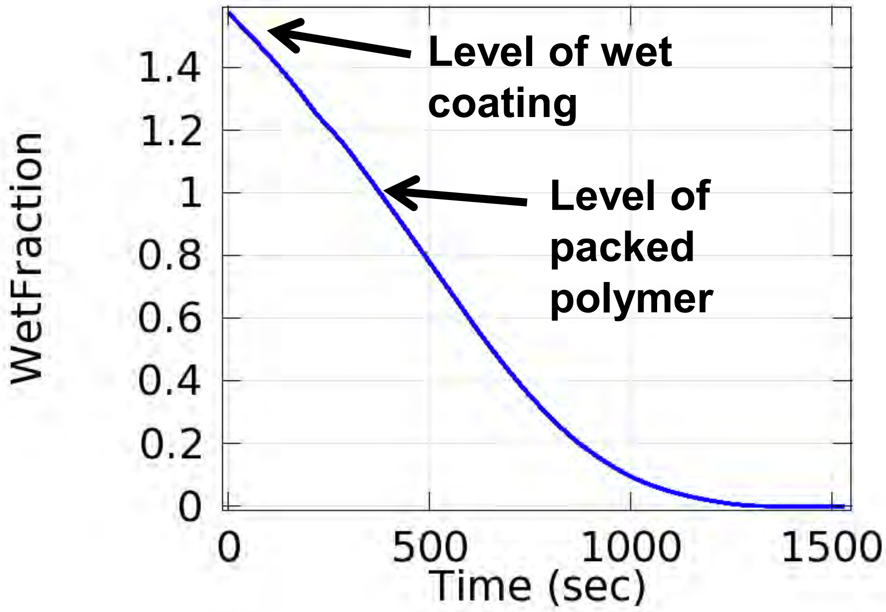
- The proved much more difficult because the boundary condition on the left is applied to a boundary which is changing in length and in material properties.

- The packed latex layer does not show up in the geometry, but as time proceeds, the incoming air runs into it.



> Average wet fraction

- **Average wet-fraction** at the interface is a good probe of the **mean level of the air-water interface**.
- Wet-fraction = (Level of Air/Water Interface)/(Height of packed polymer)
- Rate of evaporation ∝ (1-F), where F = Fill-factor
- Movement of interface per unit loss of water ∝ 1/(1-F)
- Therefore, to lowest order, the speed of interface motion is independent of F.

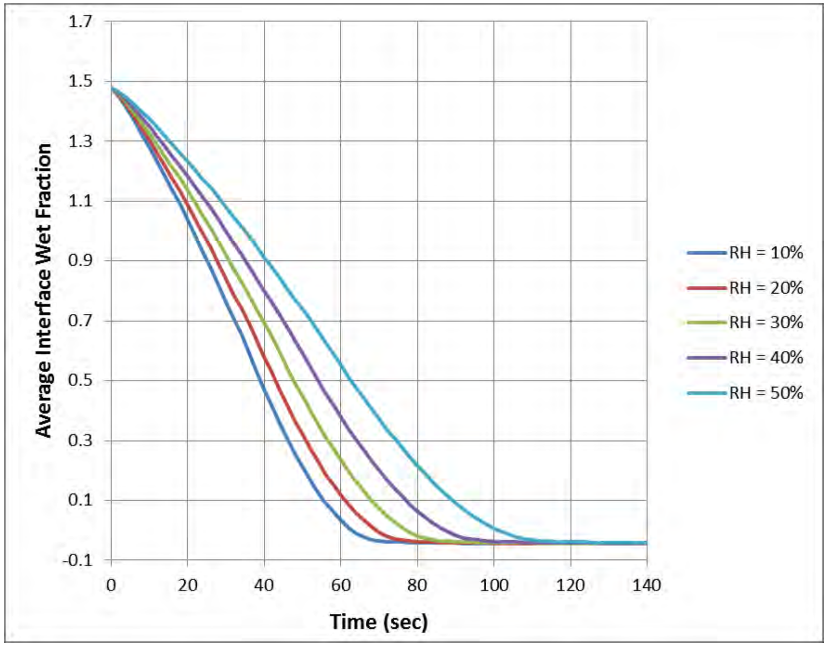


Level of wet coating

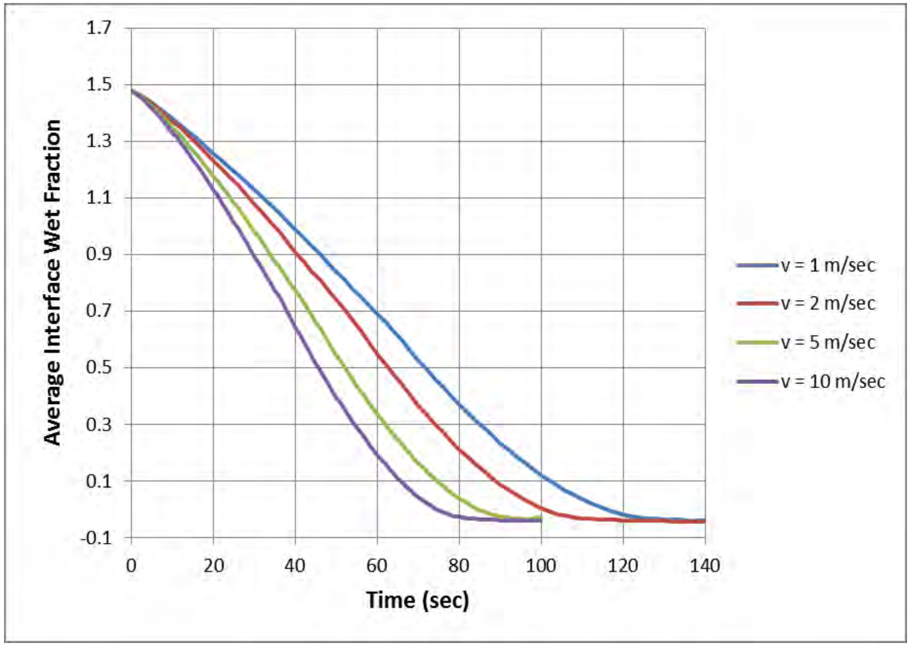
Level of packed polymer

> Evaporation vs. RH and air speed

- Length = 5 mm
- T = 345 K
- v = 2 m/sec (Air speed)

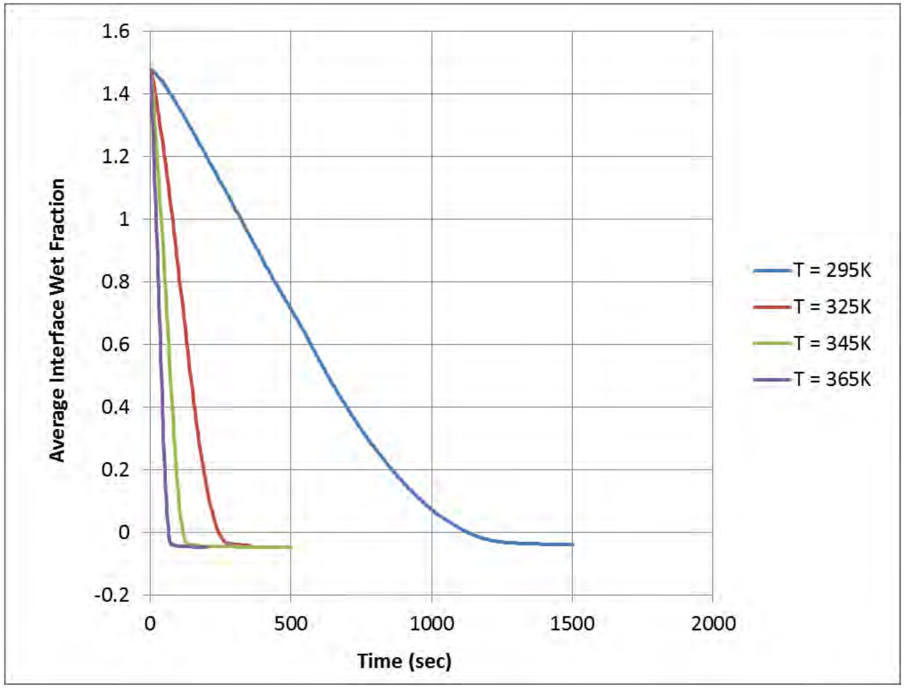


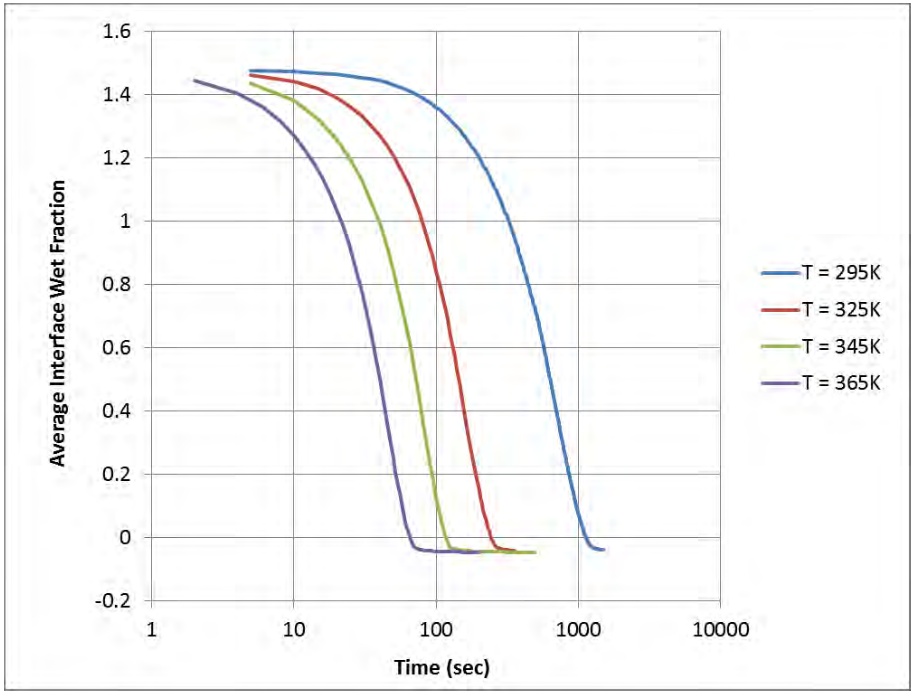
- Length = 5 mm
- T = 345 K
- RH = 50 %



> Evaporation vs. air temperature

- v = 2 m/sec (Air Speed)
- RH = 50 %
- Length = 5 mm

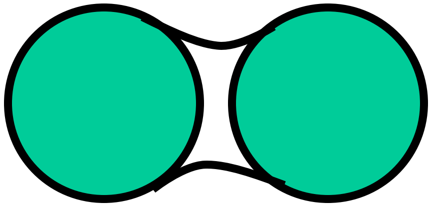




Log Scale

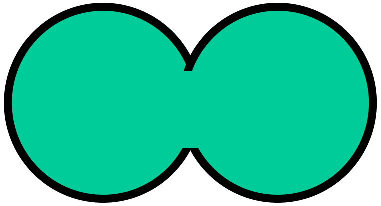
> Next steps

- **Add model of coalescence**
  - At final stage of drying, latex particles are pulled together by capillary force of water bridges. Overcomes latex stabilization forces.



Wet Sintering

  - When particles merge and water dries, their own surface tension pulls them together



Dry Sintering

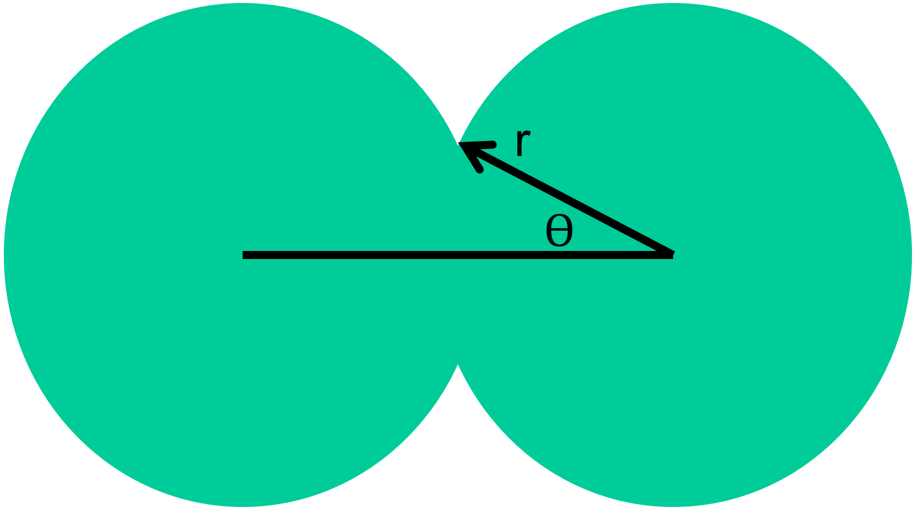
  - A model that computes the viscous flow of a unit cell of the latex pack could give the fill-factor as a function of time.   The viscosity is temperature dependent.

> Detail

Dry Sintering – Frenkel
(J. Phys. (USSR) *9*, 385,1943)

$$\theta = \frac{3\gamma t}{2\pi\eta r}$$

γ = Surface Tension
η = Polymer Viscosity
r = Particle radius
t = time



Williams, Landel and Ferry Eqn:
(J. Amer. Chem. Soc. *77*, 3701, 1955)

$$\ln(\eta) = 27.6 - \frac{40.2(T - T_g)}{51.6[K] + (T - T_g)}$$

η = Viscosity in Pa-s
T_g = Glass transition temperature in deg K
T = Temperature in deg K

> Conclusion

- **We have made a 2D model of latex drying. The model is simplified by treating all materials as "porous".**

- **Results have been obtained for two types for dryer**
  - Spraying dry air from a slot
  - Laminar flow of dry air

- **The models reveal an air/water interface profile that moves in the direction of air-flow**

- **Preliminary results have been obtained for the effects of:**
  - Temperature
  - RH
  - Air speed
  - Sample length

- **Future work will include the coalescence of the polymer**