Study Group Mathematics with Industry 2009

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Outline

About SWI 2009

- **Idea of SWI:**
  One week a group of 50 to 80 mathematicians come together to tackle industrial problems. Six companies present their problems on Monday. The group of mathematicians then devote the entire week aiming for solutions of the problems. By Friday the groups present their solution.
- **More information:**
  Problems Location Programme Participants Pictures Proceedings
- European Study Group with Industry (ESGI) 2010
  Centre for Mathematics and Computer Science (CWI), Amsterdam (The Netherlands), January 25-29

DSM Problem: Stiffening while drying

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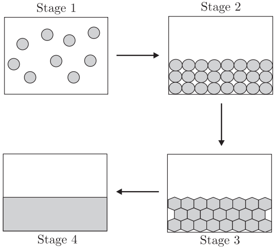
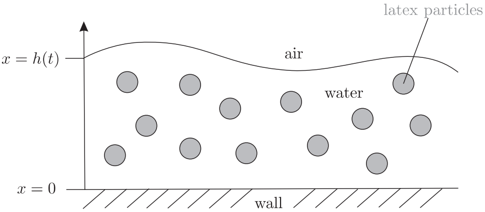
Problem description



Problem: longer drying time of waterborne paint makes it more prone to damage in the wet phase ⇝ understanding and control of drying and stiffening of waterborne coatings

Goal: development of a mathematical model of the drying and stiffening process of a paint layer

Preliminary Model: Drying



- shrinkage of the wet paint layer due to water evaporation
- h: thickness of the paint layer
- p: latex particle volume fraction
- w: water volume fraction

Preliminary Model: Drying

- derivation of a 1 D model:

$$\begin{aligned} p(x,t) + w(x,t) &= 1 \\ p_t(x,t) &= (Dp_x(x,t))_x \\ w_t(x,t) &= (Dw_x(x,t))_x \end{aligned}$$

- boundary conditions:

$$w_x(0,t) = 0 \qquad p_x(0,t) = 0$$

$$\begin{aligned} -\alpha(w(h(t),t) - Hw_{amb}) &= \frac{d}{dt}\int_0^{h(t)} w(x,t)\,dx \\ &= h'(t)w(h(t),t) + Dw_x(h(t),t) \\ 0 = \frac{d}{dt}\int_0^{h(t)} p(x,t)\,dx &= h'(t)(1 - w(h(t),t)) - Dw_x(h(t),t) \end{aligned}$$

- for $0 < x < h(t)$ and $t > 0$

Preliminary Model: Drying

- system of equations for the volume fraction w with layer thickness h:

$$
\begin{aligned}
w_t(x,t) &= (D w_x(x,t))_x \\
w_x(0,t) &= 0 \\
w_x(h(t),t) &= -\frac{\alpha}{D}(w(h(t),t) - Hw_{amb})(1 - w(h(t),t)) \\
w(x,0) &= w_0(x) \\
h'(t) &= -\alpha(w(h(t),t) - Hw_{amb}) \\
h(0) &= h_0
\end{aligned}
$$

- for $0 < x < h(t)$ and $t > 0$

Preliminary calculations

- moving boundary is transformed into a fixed one by introducing the new variables $\xi = \frac{x}{h(t)}$ and $\tau = t$
- hence

$$\frac{\partial}{\partial x} = \frac{\partial \xi}{\partial x}\frac{\partial}{\partial \xi} + \underbrace{\frac{\partial \tau}{\partial x}}_{=0}\frac{\partial}{\partial \tau} = \frac{1}{h(t)}\frac{\partial}{\partial \xi}$$

$$\frac{\partial}{\partial t} = \frac{\partial \xi}{\partial t}\frac{\partial}{\partial \tau} + \underbrace{\frac{\partial \tau}{\partial t}}_{=1}\frac{\partial}{\partial \tau} = -\frac{\xi h'(t)}{h(t)}\frac{\partial}{\partial \xi} + \frac{\partial}{\partial \tau}$$

Preliminary calculations

- physical transport model (writing $t = \tau$)

$$\begin{aligned}
w_t(\xi, t) &= \frac{\xi h'(t)}{h(t)} w_\xi(\xi, t) + \left(\frac{D}{h^2(t)} w_\xi(\xi, t) \right)_\xi \\
w_\xi(0, t) &= 0 \\
w_\xi(1, t) &= -\frac{\alpha h(t)}{D} (w(1, t) - H w_{amb})(1 - w(1, t)) \\
w(\xi, 0) &= w_0(\xi) \\
h'(t) &= -\alpha (w(1, t) - H w_{amb}) \\
h(0) &= h_0
\end{aligned}$$

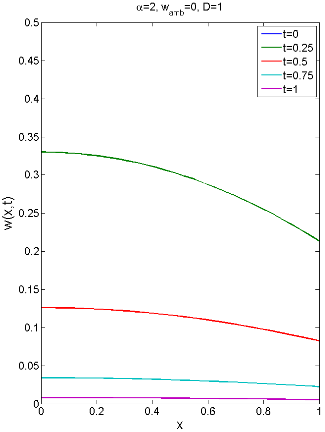
- for $0 < \xi < 1$ and $t > 0$

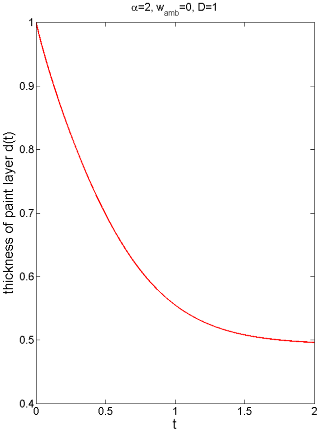
Preliminary calculations

- using the method of lines (spatial semi-discretization), the system of PDEs is approximated by a system of ODEs
- numerical solution can be obtained with standard procedures in MATLAB™
- $w(x_0,t) = w(x_2,t)$, $w_i := w(x_i,t)$, $h = \frac{1}{n-1}$, $\Delta w_i := w_i - w_{i-1}$

$$\frac{d}{dt}\begin{pmatrix} w_1 \\ \vdots \\ w_i \\ \vdots \\ w_n \\ d(t) \end{pmatrix} = \begin{pmatrix} \frac{D(w_1)\Delta w_2 - D(w_2)\Delta w_1}{d^2(t)h^2} \\ \vdots \\ \frac{D(w_i)\Delta w_{i+1} - D(w_{i-1})\Delta w_i}{d^2(t)h^2} - \alpha\frac{(w_n - w_{amb})(i-1)\Delta w_i}{d(t)} \\ \vdots \\ \frac{-d(t)\alpha(w_n - w_{amb})h - D(w_n)\Delta w_n}{d^2(t)h^2} - \alpha\frac{(w_n - w_{amb})(n-1)\Delta w_n}{d(t)} \\ -\alpha(w_n - w_{amb}) \end{pmatrix}$$

Preliminary calculations





Improvement of the Model: Outlook

- coagulation of 2 latex particles
- coagulation of the arbitrary number of particles (cluster formation)
- concept of "Stiffness"
- varying diffusion coefficient
  $D = D(\text{size of cluster}, \text{water volume fraction})$
- "Film" formation
- possible extension of the model to 2D

Model for the coagulation of 2 latex particles

- derivation of a 1 D model:

$$\begin{aligned} p_t(x,t) &= -cp^2(x,t) + (D_p p_x(x,t))_x \\ q_t(x,t) &= \frac{1}{2}cp^2(x,t) + (D_q q_x(x,t))_x \\ w_t(x,t) &= -(D_p p_x(x,t))_x - 2(D_q q_x(x,t))_x \end{aligned}$$

- boundary conditions:

$$\begin{aligned} w_x(0,t) = p_x(0,t) = q_x(0,t) &= 0 \\ h'(t)p(h(t),t) + D_p p_x(h(t),t) &= 0 \\ h'(t)q(h(t),t) + D_q q_x(h(t),t) &= 0 \\ h'(1-p-2q) - D_p p_x - 2D_q q_x &= -\alpha(1-p-2q-w_{amb}),\ x = h(t) \end{aligned}$$

- for $0 < x < h(t)$ and $t > 0$

Model for the arbitrary cluster size

- full set of equations now reads

$$
\begin{aligned}
P_t(n,x,t) &= (D_n P_x(n,x,t))_x - A(n,x,t) + B(n,x,t) \\
P_x(n,0,t) &= 0 \\
D_n P_x(n,h(t),t) &= -h'(t)P(n,h(t),t) \\
w(x,t) &= 1 - \sum_{n=1}^{N} nP(n,x,t) \\
h'(t) &= -\alpha(w(h(t),t) - Hw_{amb})
\end{aligned}
$$

- for $0 \leq x \leq h(t)$ and $t > 0$
- $nP(n,x,t)$ - joint volume fraction of the clusters of size n

Model for the arbitrary cluster size

$$A(n,x,t) = \sum_{m=1}^{N-n} C_{n,m} P(n,x,t) P(m,x,t) \quad \text{(dissipation rate)}$$

$$B(n,x,t) = \frac{1}{2} \sum_{m=1}^{n-1} C_{n,n-m} P(m,x,t) P(n-m,x,t) \quad \text{(generation rate)}$$

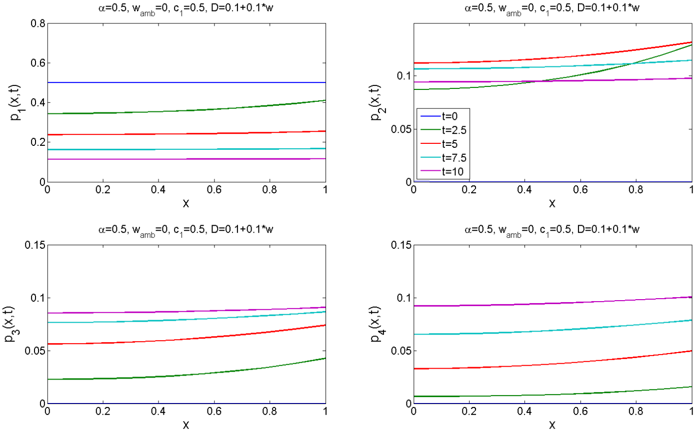
$$D_n = \frac{1}{n} D_1(w)$$

Modeling of S: **Stiffness**

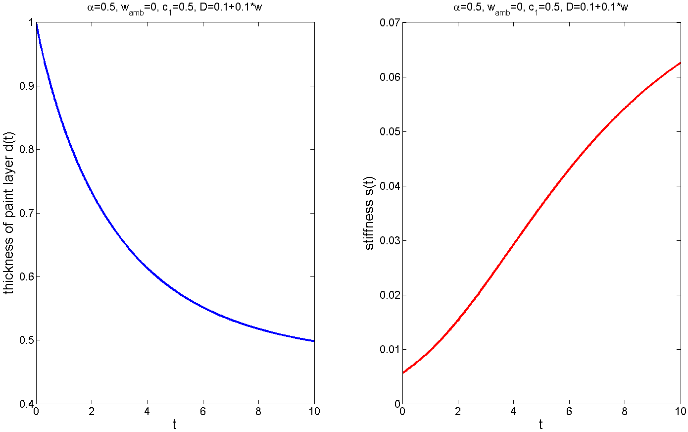
$$S_{local}(x,t) = \sum_{k=1}^{N} k^2 P(k,x,t)$$

$$\frac{1}{S(t)} = \frac{1}{h(t)} \int_0^{h(t)} \frac{1}{S_{local}(x,t)} \,\mathrm{d}x$$

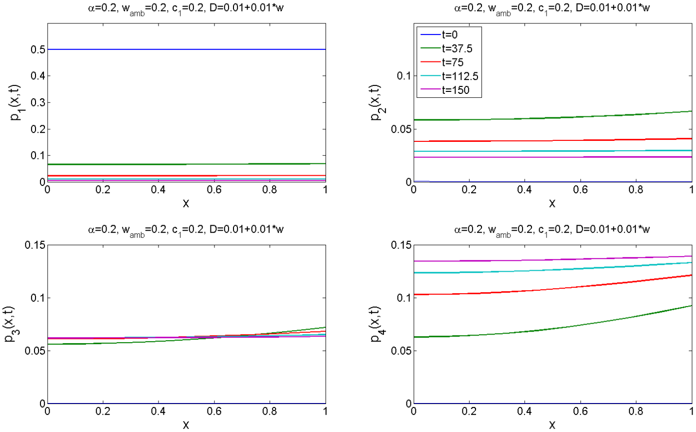
Numerical Calculations



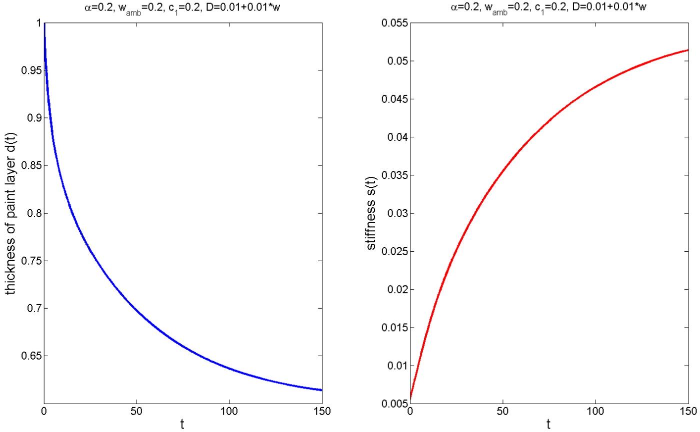
Numerical Calculations



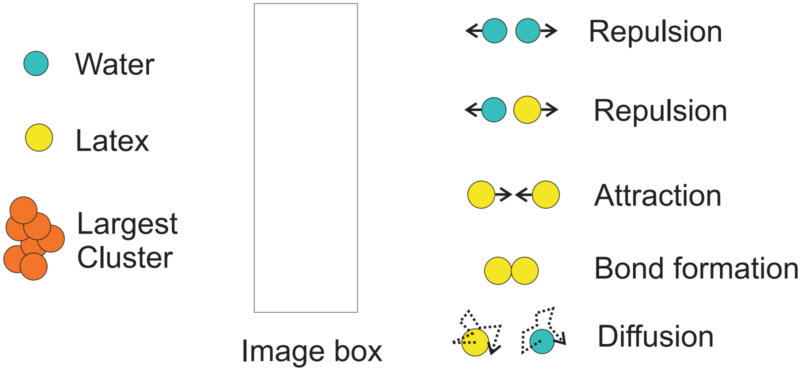
Numerical Calculations



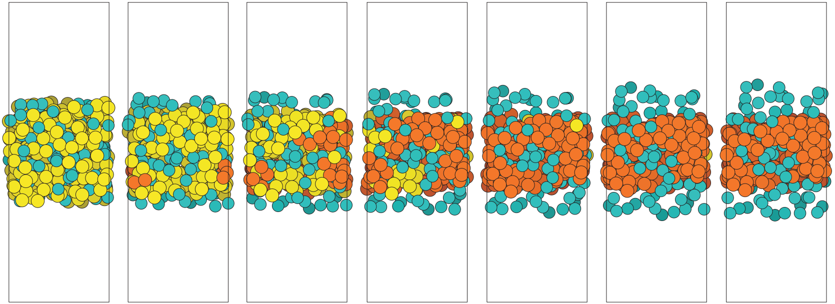
Numerical Calculations



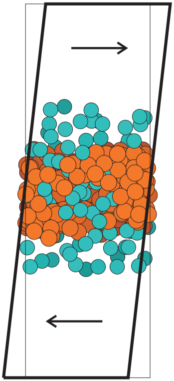
Direct Molecular Simulation



Direct Molecular Simulation



Direct Molecular Simulation



Summary and Future Direction

- two approaches for the understanding of the drying and stiffening process of the paint
- direct molecular simulations and the numerical studies of the model have been performed
- model for the "Stiffening While Drying" of the paint has been proposed
- coagulation process of the latex particles has been incorporated
- possible extension: Stress driven water flow, cracking, two dimensional flow, physics of film formation process, non-dimensionalisation

References

- S.D. Howinson et al.
  - A mathematical model for drying paint layers
- A.F. Routh and W.B. Russel
  - Horizontal Drying Fronts During Solvent Evaporation from Latex Films
  - Deformation Mechanisms during Latex Film Formation
- B.W. van de Fliert and R. van der Hout
  - A free boundary problem for evaporating layers
  - Stress-driven diffusion in a drying liquid paint layer
  - A generalized Stefan problem in a diffusion model with evaporation

Thank you for your attention.