A Numerical Model of Bubbling Thermoplastics

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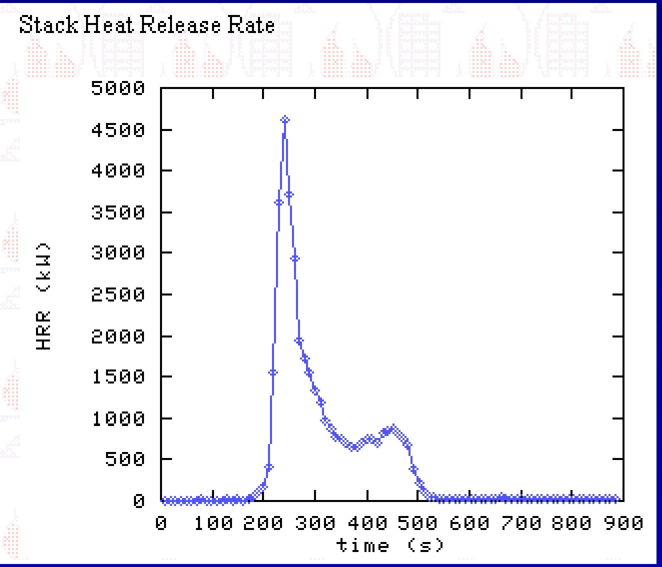
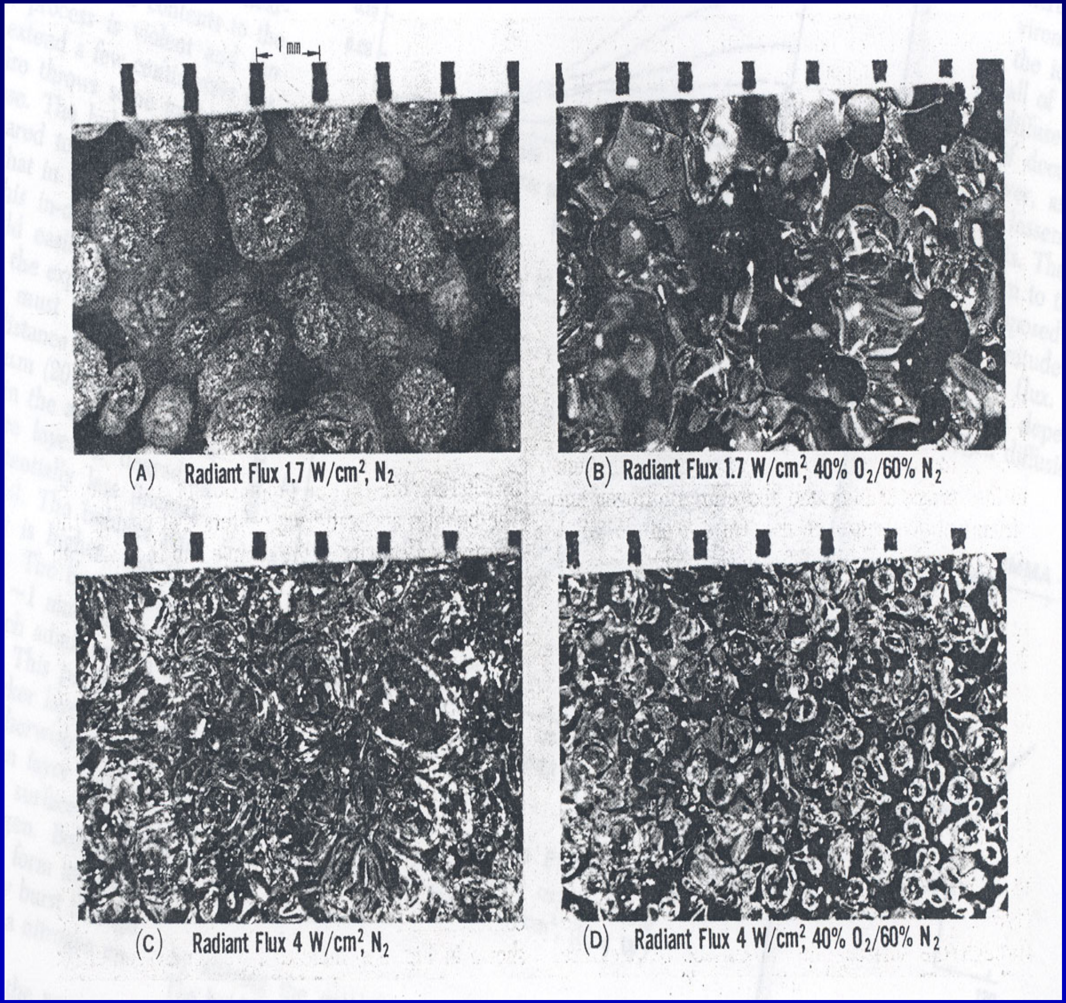
Thermoplastic Materials in Fire



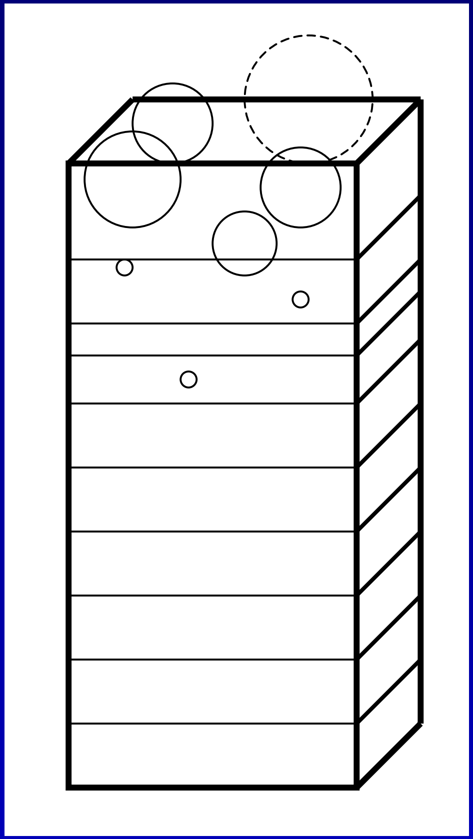
Microscopic Photographs of PMMA



Kashiwagi and Ohlemiller, 19th Intl. Symp. on Comb., pp. 815-823 (1982)

Numerical Model

- 1-D Finite element model
  - Mass balance for gas and polymer
  - Energy balance
- Individual bubble dynamics
  - In 3-D
  - Sizes and locations of bubbles determine amount of gas in each element
  - Motion of bubbles determine velocities



Continuity Equations

- Polymer

$$\frac{\partial}{\partial t}\left(\rho_p \phi_p\right) + \frac{\partial}{\partial z}\left(\rho_p \phi_p W_p\right) = -\rho_p \phi_p B e^{-E/RT}$$

- Gas

$$\frac{\partial}{\partial t}\left(\rho_g \phi_g\right) + \frac{\partial}{\partial z}\left(\rho_g \phi_g W_g\right) = +\rho_p \phi_p B e^{-E/RT}$$

- Volume Fractions: $\phi_p = \frac{V_p}{V}$ $\qquad \phi_g = \frac{V_g}{V}$

Energy Equation

$$(\rho c_p)^* \left(\frac{\partial T}{\partial t} + W^* \frac{\partial T}{\partial z} \right) = \frac{\partial}{\partial z} \left(k^* \frac{\partial T}{\partial z} \right) - H_v \rho_p \phi_p B e^{-E/RT}$$

where

$$(\rho c_p)^* = \sum_k \rho_k \phi_k c_{p_k}$$

$$W^* = \frac{\sum \rho_k \phi_k W_k}{\sum \rho_k \phi_k}$$

$$k^* = (k_p)^{\phi_p} (k_g)^{\phi_g}$$

Bubble Model

- Nucleation
- Bubble growth
- Migration
- Coalescence
- Bursting

Bubble Nucleation

- Homogeneous vs. heterogeneous nucleation
  (Thermal fluctuations) (Impurities)

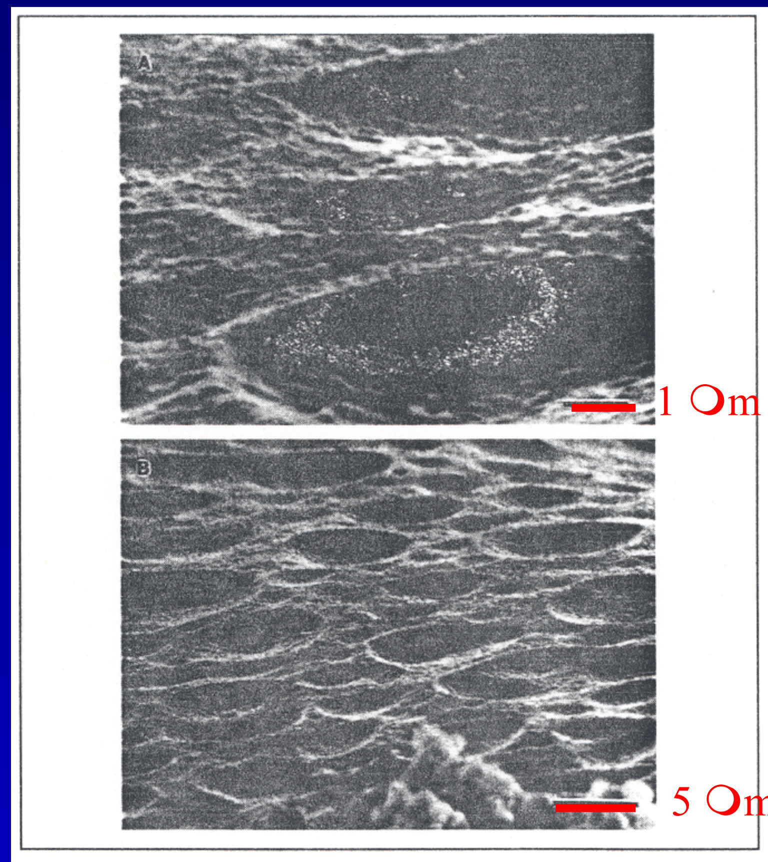
- Arrhenius function for nucleation rate J

$$J = MB\exp\left(-\Delta F_{cr} / k_B T\right)$$

  - Elasticity
  - Gas diffusivity through melt

- Rate easily varies by 9+ orders of magnitude!

Secondary Nucleation



Yarin et al., AIChE J. 45:2590-2605 (1999)

Bubble Growth

- Models
  - Infinite domain; finite radius
  - Temperature gradients – radial
  - Dominant mechanism depends on size
    - Surface tension, inertia, evaporation
  - Diffusion-driven: $R \propto t^{1/2}$
  - Polymer melt: between Newtonian fluid and diffusion-driven growth
- Secondary nucleation
  - In strongly viscoelastic liquids

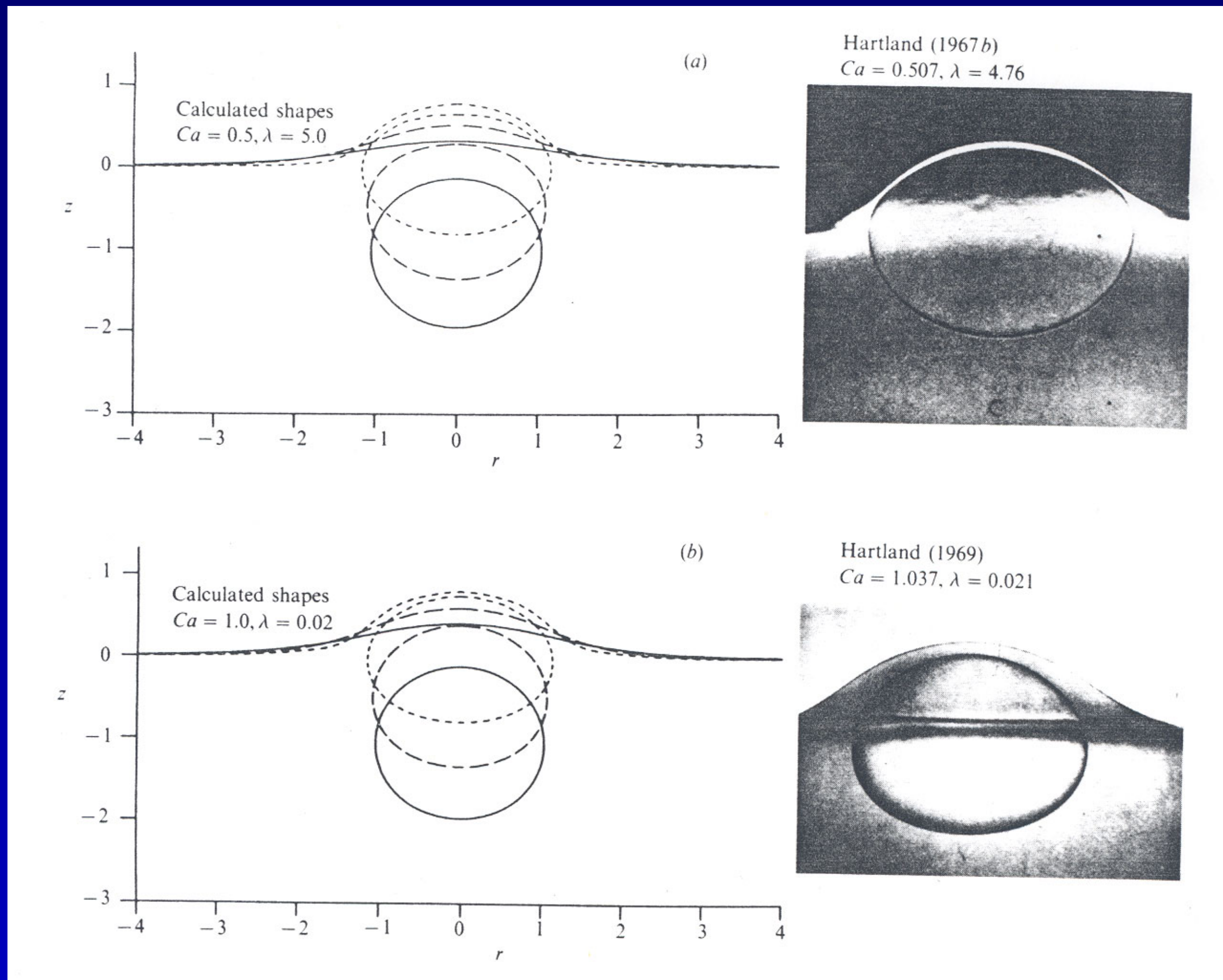
Bubble Migration

- Driven by gravity, temperature gradients (surface tension, viscosity dependence on T)

$$U = -\frac{2(\rho_p - \rho_g)gR^2}{9\mu} + \left[2R\dot{R}\left(-\frac{d\ln\mu}{dT}\right) + \frac{R}{3\mu}\left(-\frac{d\ln\sigma}{dT}\right)\right]\frac{\partial T}{\partial z}$$

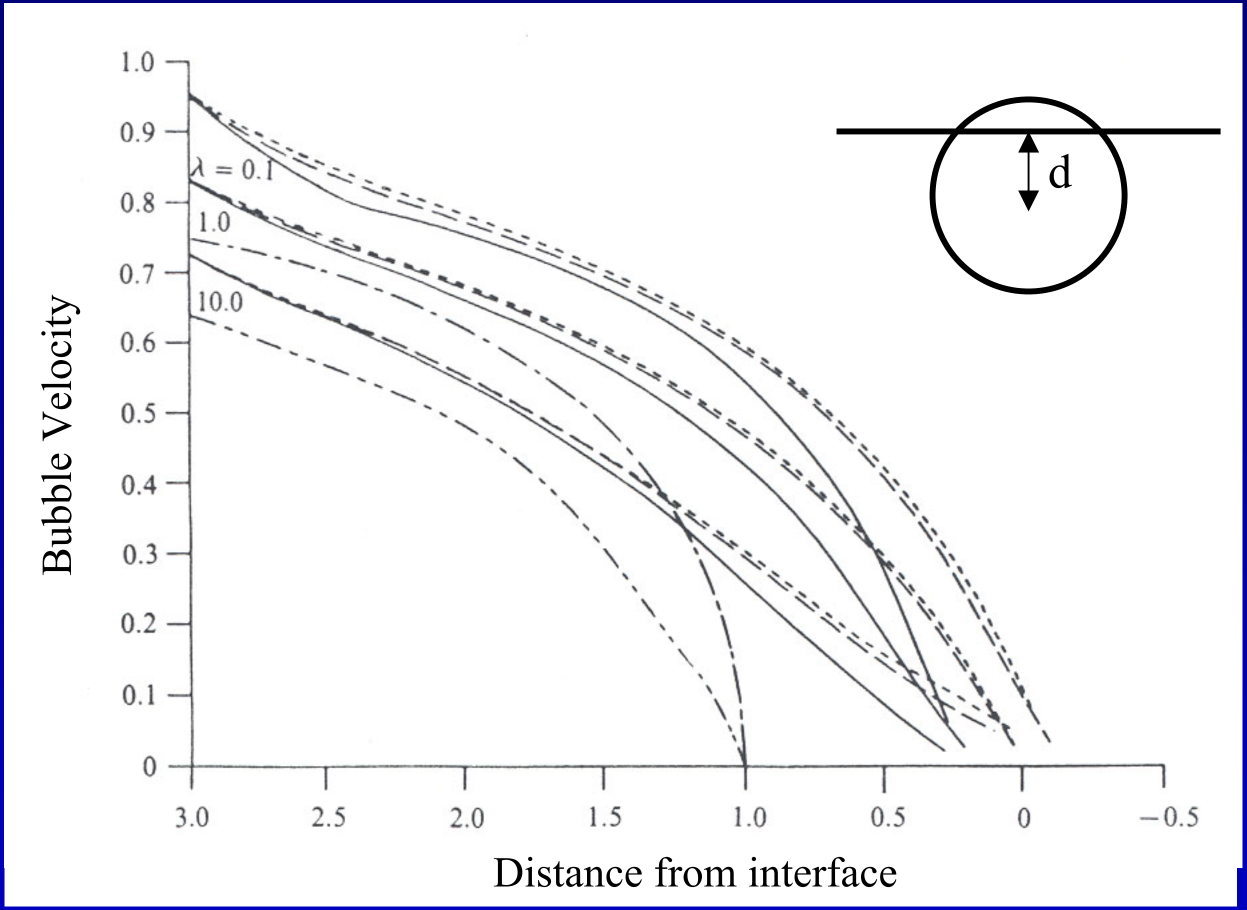
- Wake effects
- Bubbles slow as approach surface

Approach to Interface



Chi and Leal, J. Fluid Mech. 201:123-146 (1989)

Bubble Velocity Nearing Interface

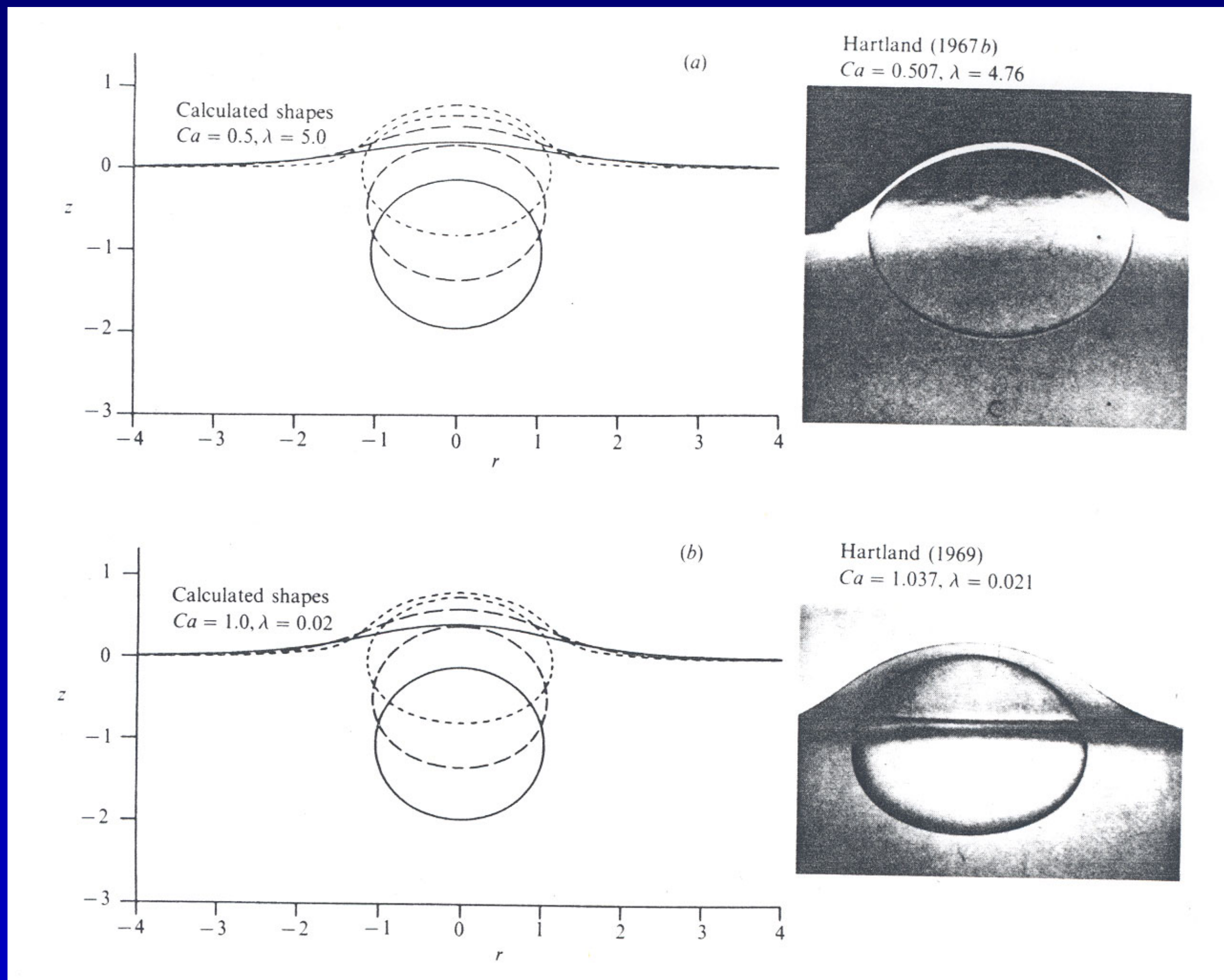


Chi and Leal, J. Fluid Mech. 201:123-146 (1989)

Coalescence and Bursting

- Stages:
  - Approach
  - Drainage of thin film
  - Rupture by surface instability - rapid
- Strongly dependent on presence of surfactants
  - Clean interface: ~ 1 ms
  - Surfactant: ~100 s
- Vaporization due to heating not considered

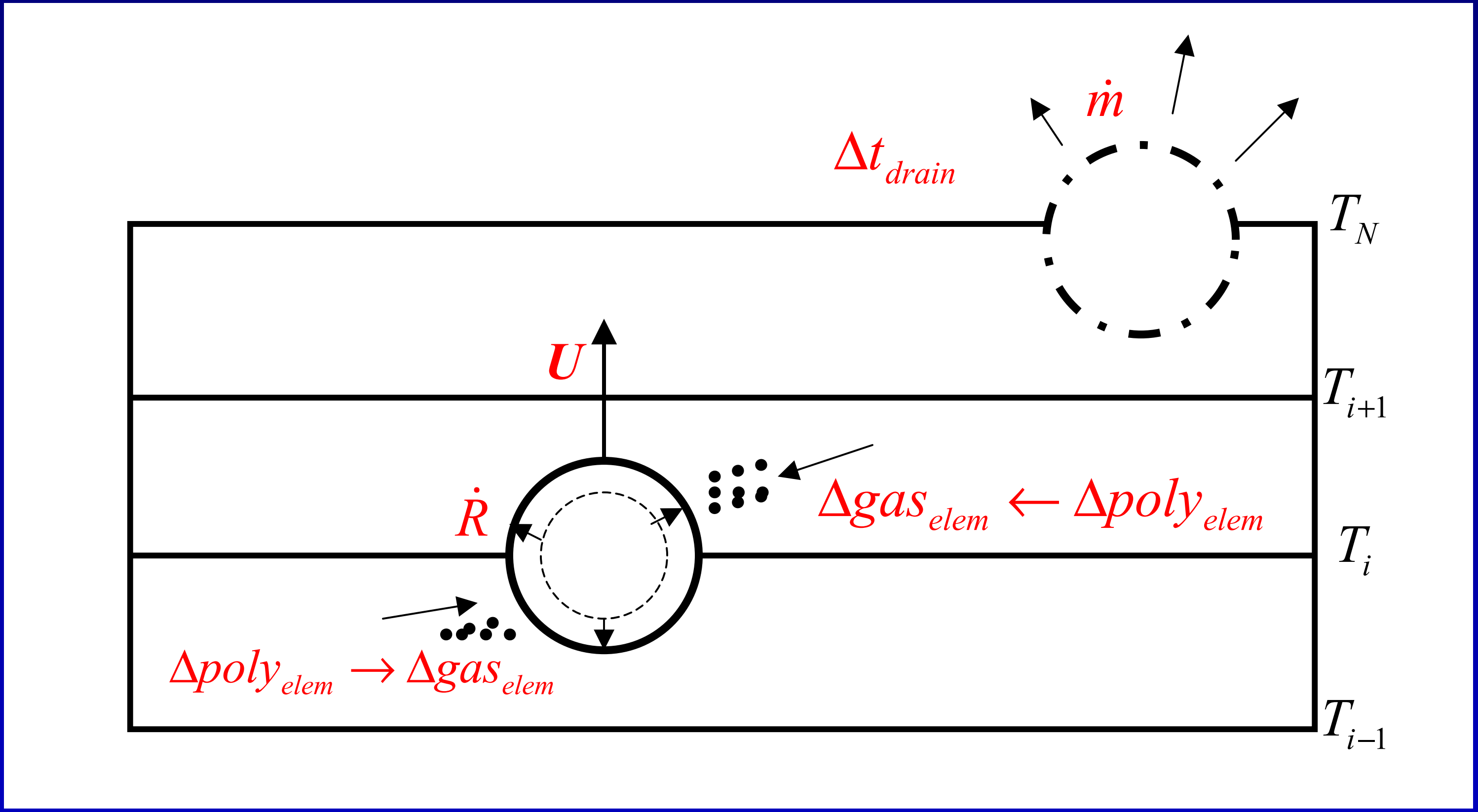
Thin-film Drainage



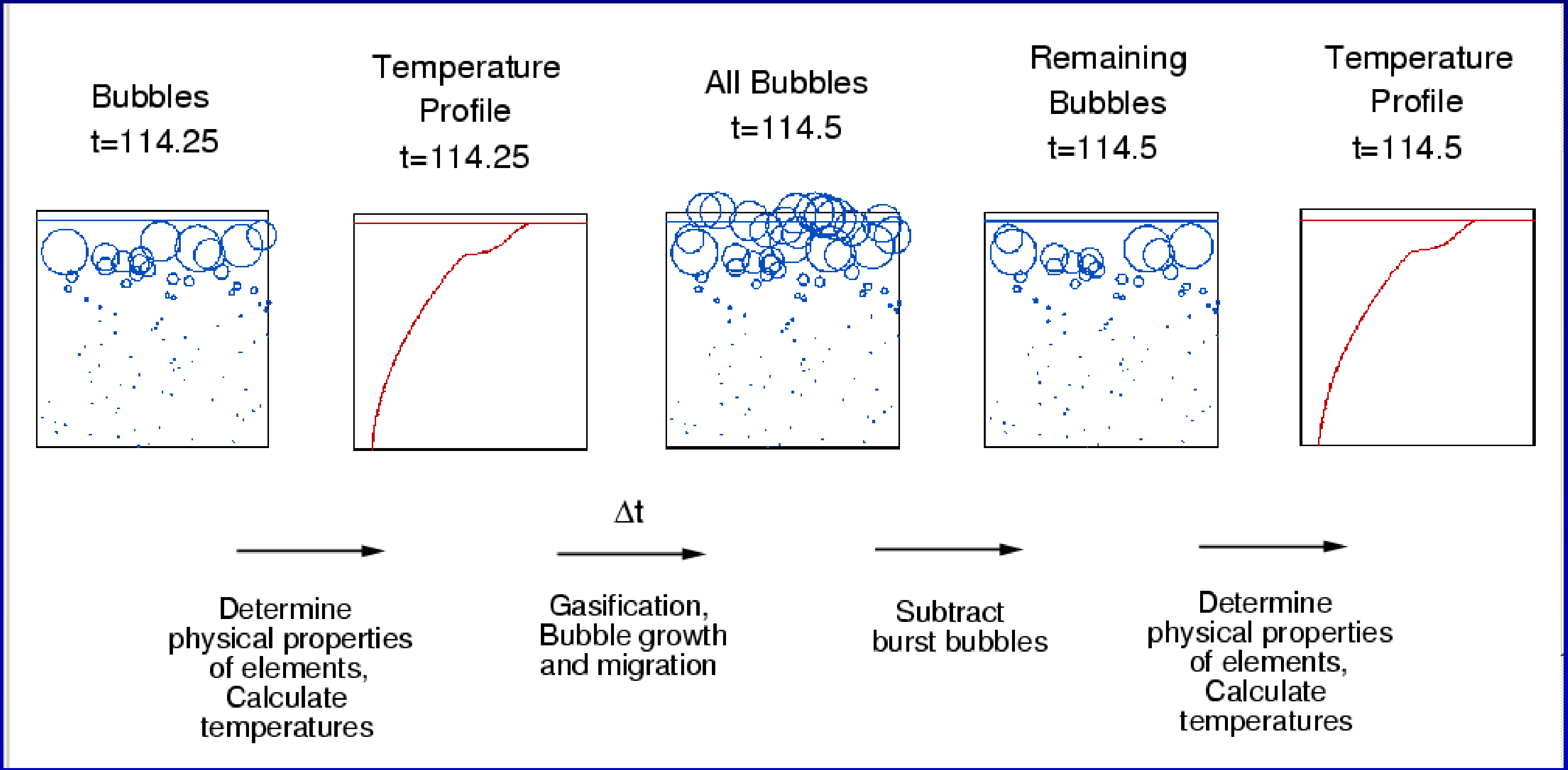
Bursting

- Gases released by sample
  - Determines the mass loss rate
  - Heat release rate of fire
- Long-lasting bubbles may form insulating layer

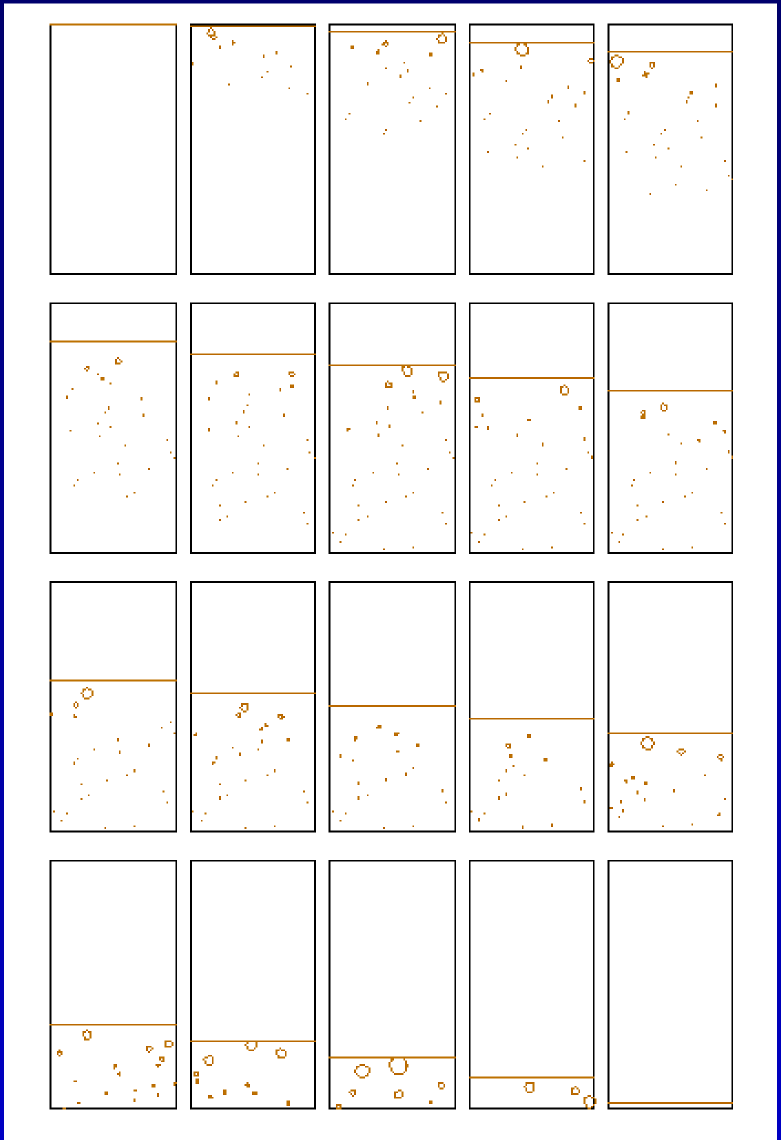
Bubble Model



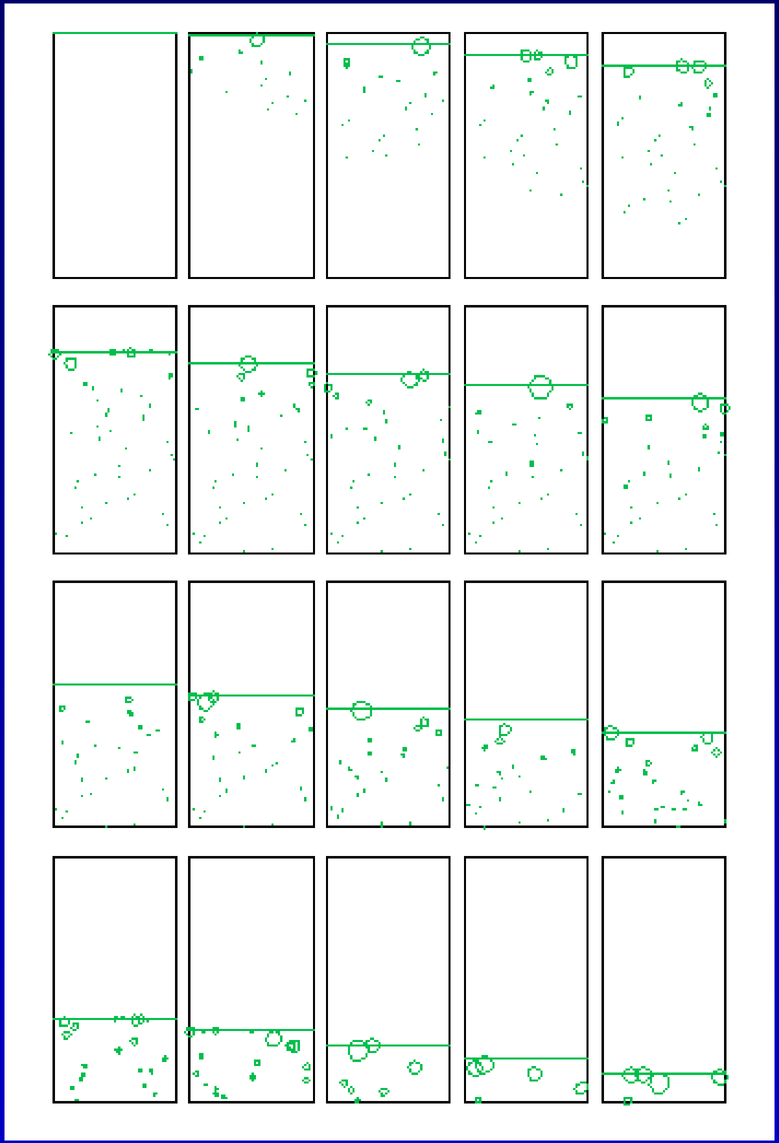
Numerical Model



Effects of Bursting Delay in PP

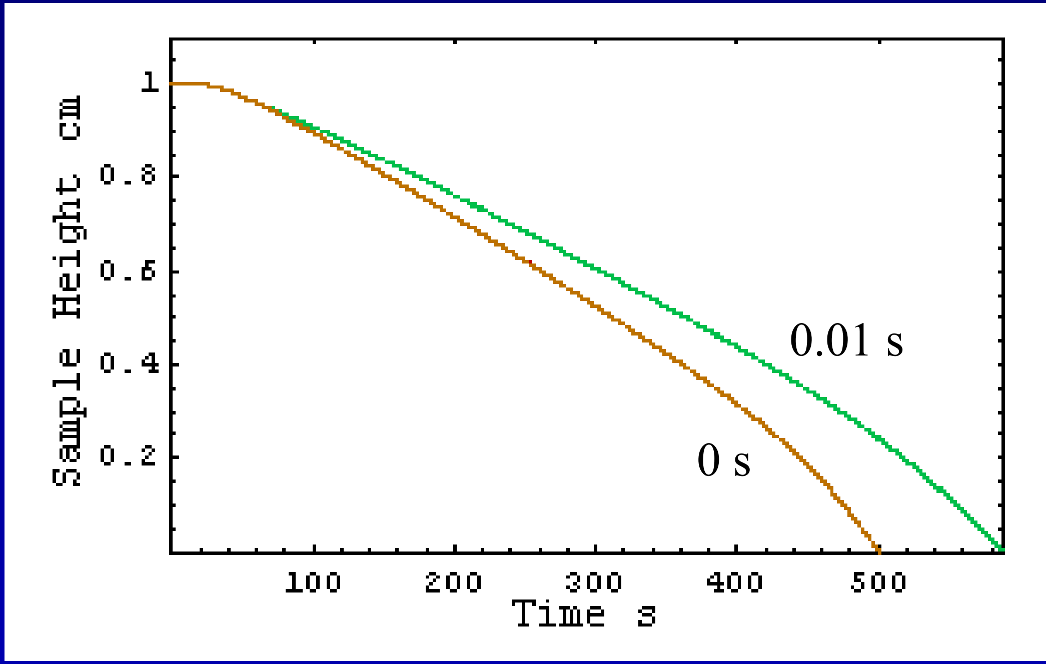


Drainage time = 0 sec



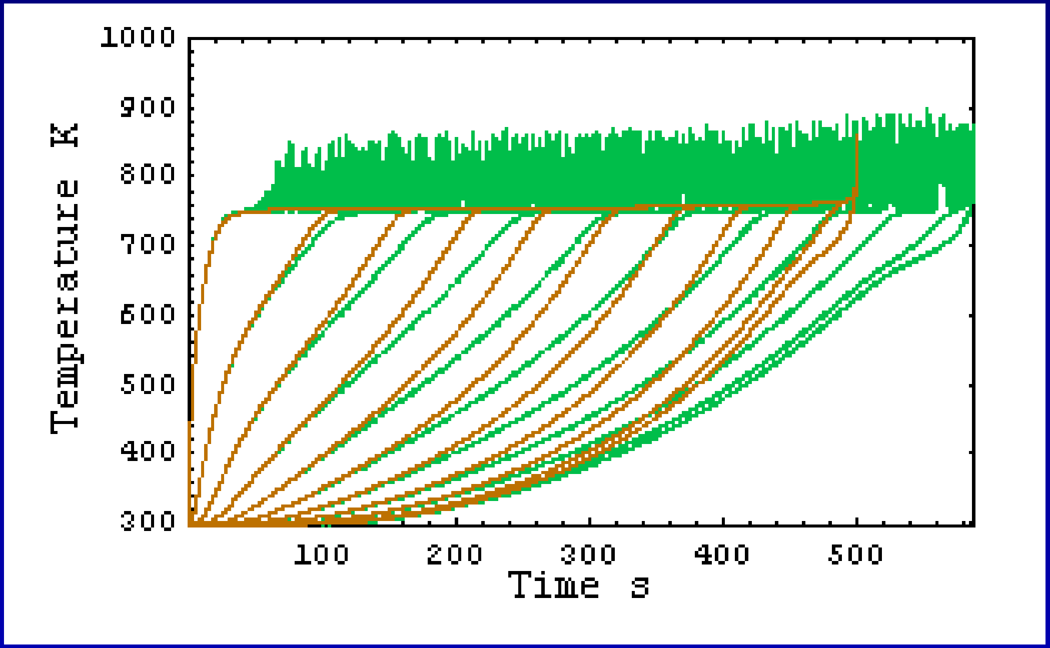
0.01 sec

Effect of Bursting Delay on Sample Thickness vs. Time



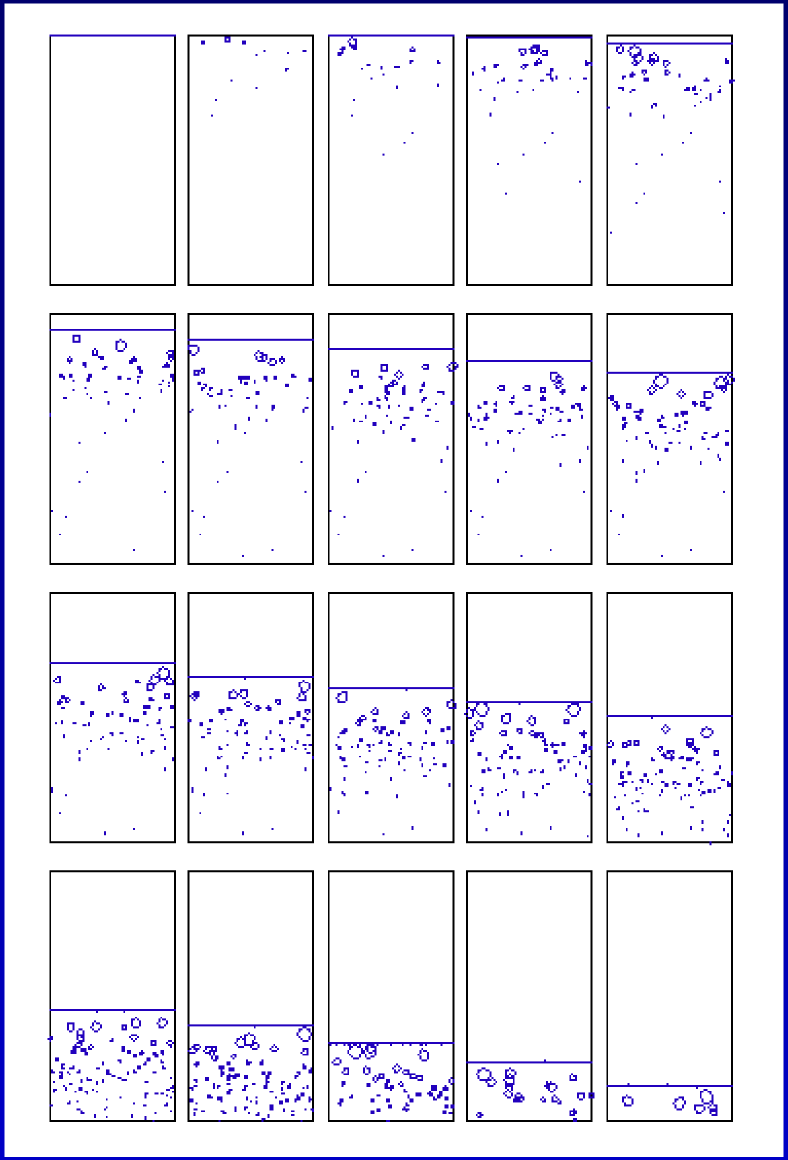
Drainage times = 0, 0.01 seconds

Temperature vs Time for Sample Surfaces

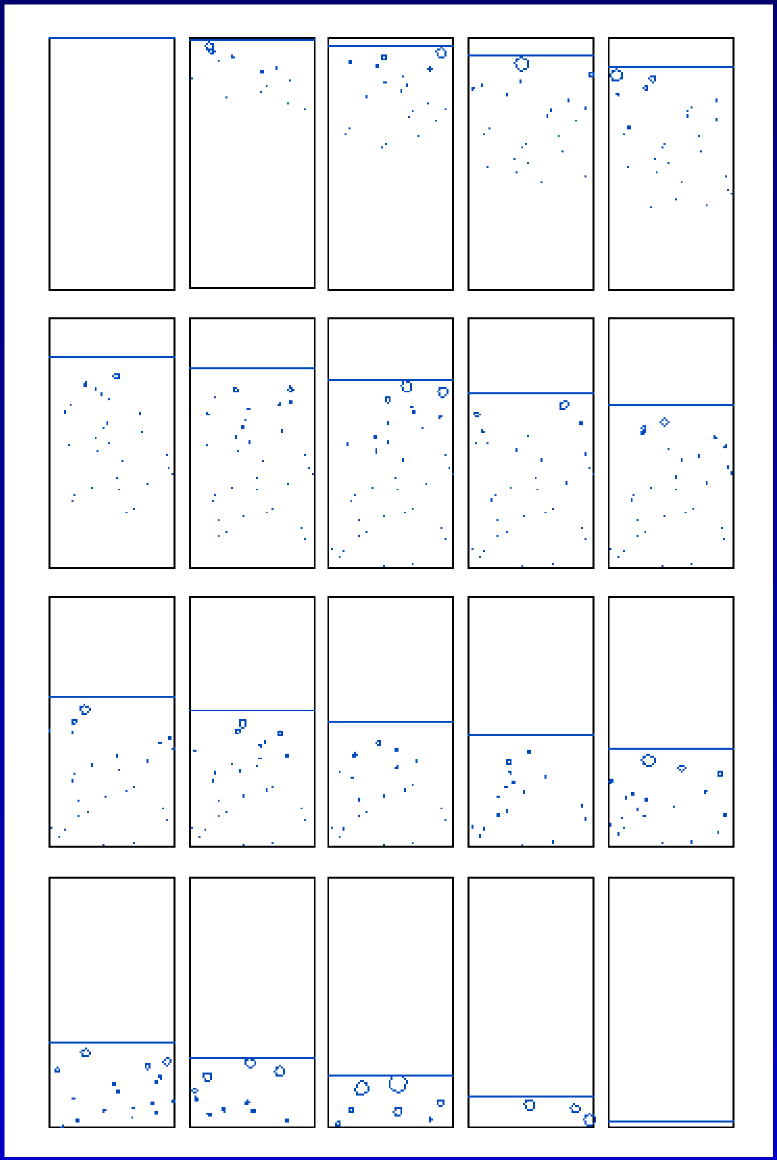


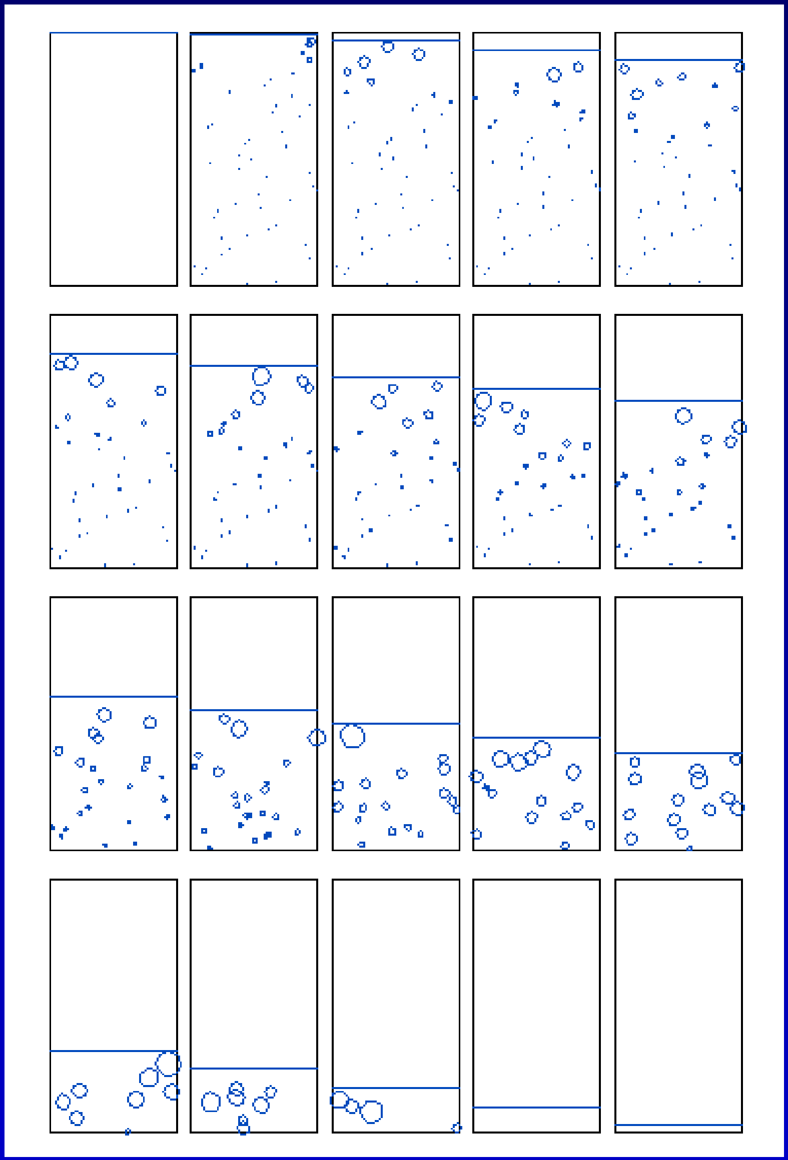
Drainage times = 0 (orange), 0.01 (green) seconds

Nucleation Model



PP vs. PMMA





Other Bubble Effects

- Radiation
  - Internal transmission
  - Scattering
- Oxygen entrainment
- Distortion of surface geometry

Conclusions

- Bubbling behavior in thermoplastic materials exposed to fire is highly complex
  - First principle modeling has a long way to go
- Because of insulating layer and direct impact on mass loss rate, bubble behavior at surface is critical
  - Bursting, coalescence, nucleation, approach to interface
  - Need to include radiation effects