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Benchtop Experimental and Computational Design Tools for Continuous Drying Processes

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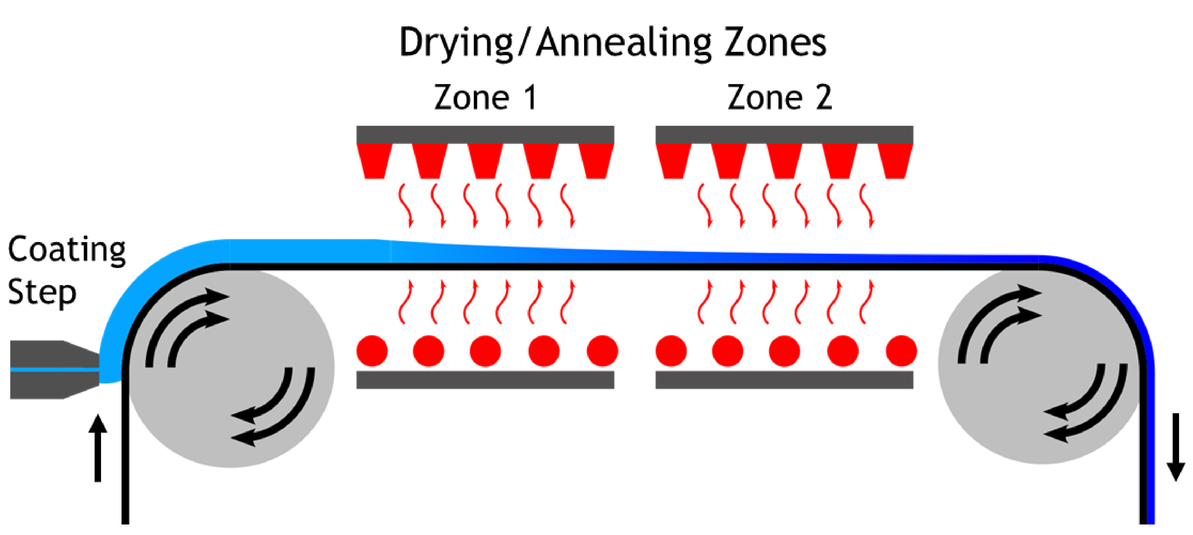
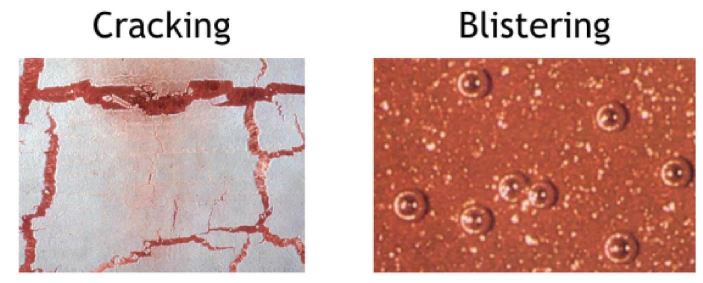
Continuous Coating and Drying Processes





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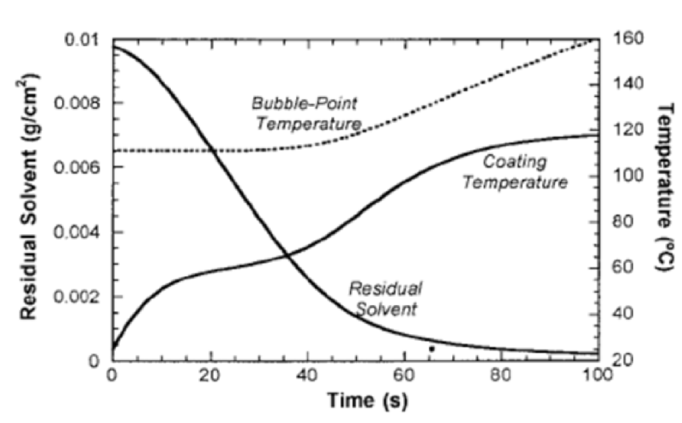
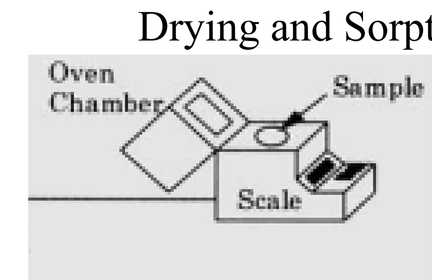


Price Jr. & Cairncross, J. Appl. Polym. Sci. 2000. 78, 149

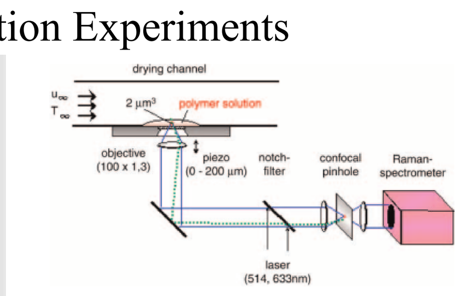
- Continuous coating and drying processes key manufacturing process
- Defects may arise for poor drying conditions, limiting process throughput
- Necessary to obtain key thermodynamic and diffusivity model parameters for drying oven design

Drying Process Design: Prior Work and Challenges

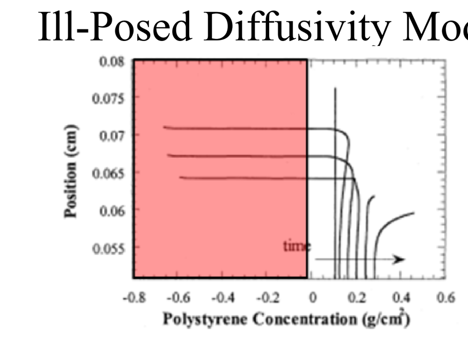
Drying and Sorption Experiments



Price Jr. et al. AIChE J. 1997. 43, 1925

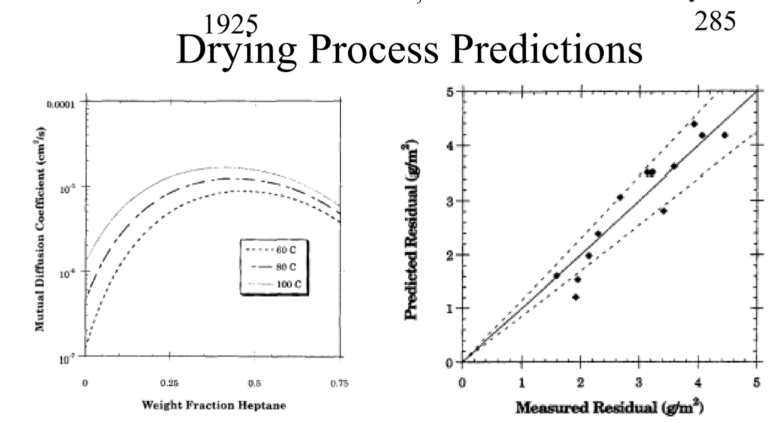

Schabel et al. Dry. Technol. 2004. 22, 285

Ill-Posed Diffusivity Models



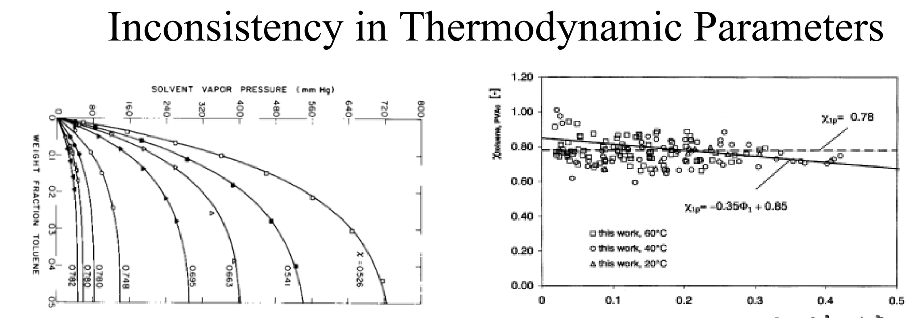
Price Jr. & Romdhane. AIChE J. 2003. 49, 309

Drying Process Predictions



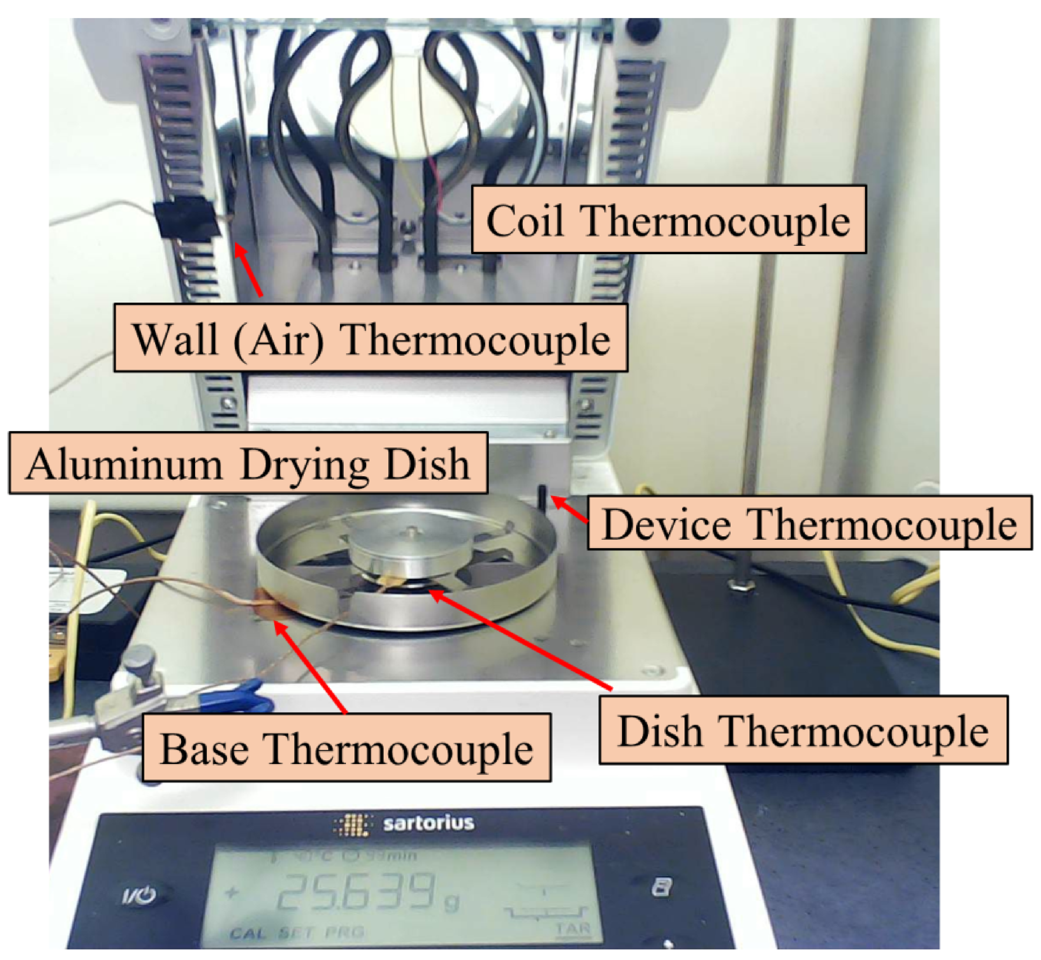
Price Jr. et al. AIChE J. 1997. 43, 1925

Inconsistency in Thermodynamic Parameters


Vrentas et al. J. Polym. Sci. B. 1985. 23, 289

Mamaliga et al.. Chem. Eng. Process. 2004. 43, 753

Benchtop Drying Apparatus



- Moisture analyzer with thermocouples and data logger provides a cost-effective drying apparatus
- Sample and surrounding temperatures may be measured and used as inputs in computational model

1D Drying Model

Heat Transfer B.C.: Liquid-Air Interface

$$\kappa \frac{\partial T}{\partial y} = \epsilon \sigma (T^4_{coil} - T^4) + h_{air}(T - T_\infty) + \sum_{i=1}^{N_{solv}} \Delta H_{vap} k_i (P_i^v - P_{0,i})$$

Drying Flux for solvent i

$$\sum_{j=1}^{N_{solv}} D_{ij} \frac{\partial c_j}{\partial y} + c_i \frac{\partial H}{\partial t} = -k_i (P_i^v - P_{0,i})$$

Vapor-Pressure: Flory Huggins

$$P_i^v(\epsilon, T) = \phi_i(\epsilon) \cdot \gamma_i(\epsilon) \cdot \bar{P}_i^v(T)$$

$$\bar{P}_i^v(T) = \exp\left(A_i - \frac{B_i}{T + C_i}\right)$$

Species Transport: Diffusion

$$\frac{\partial c_i}{\partial t} = \frac{\partial}{\partial y}\left(\sum_{j=1}^{N-1} D_{ij}(\epsilon, T) \frac{\partial c_j}{\partial y}\right)$$

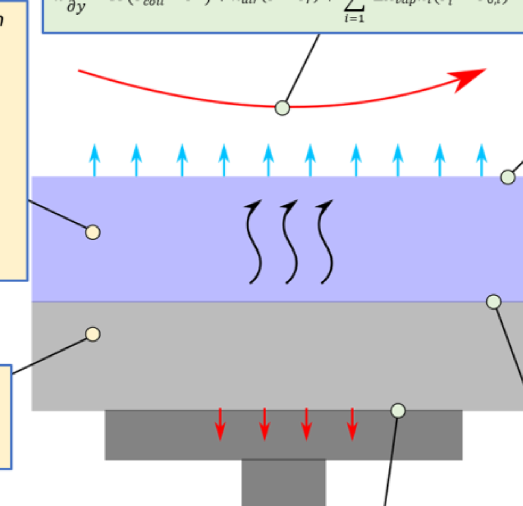
$D_{ij}(\epsilon, T)$ from Price (2004)

Heat Transfer: Liquid

$$\rho C_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial y}\left(\kappa \frac{\partial T}{\partial y}\right)$$

Heat Transfer: Substrate

$$\frac{\partial T_s}{\partial t} = \frac{\kappa_s}{\rho_s C_{p,s}} \frac{\partial^2 T_s}{\partial y^2}$$



$$\chi_{ij} = \chi_{r,ij} \frac{273.15K}{T}$$

No-Flux B.C. for solvent i

$$\sum_{j}^{N_{solv}} D_{ij} \frac{\partial c_j}{\partial y} = 0$$

Heat Transfer B.C.

$$\kappa_s \frac{\partial T_s}{\partial y} = \kappa \frac{\partial T}{\partial y}$$

$$T_s(0^+, t) = T(0^-, t)$$

Heat Transfer Boundary Condition

$$\kappa_s \frac{\partial T_s}{\partial y} = h_{base}(T_s - T_b)$$

Free-Volume Diffusivity Model

$$D_{ik} = D_i \left(\frac{c_i}{RT} \frac{\partial \mu_i}{\partial c_k}\right) - \sum_{j=1}^{N-1} D_j c_i \hat{V}_j \left(1 - \frac{D_N \hat{V}_N M_N}{D_j \hat{V}_j M_j}\right)\left(\frac{c_j}{RT} \frac{\partial \mu_j}{\partial c_k}\right)$$

$$D_i = D_{0,i} \exp\left(\frac{-\gamma \sum_{j=1}^{N} \left(\omega_j \hat{V}_j^* \frac{\xi_{iN}}{\xi_{jN}}\right)}{\hat{V}_{FH}}\right) \quad \frac{\hat{V}_{FH}}{\gamma} = \sum_{j=1}^{N} \frac{K_{1i}}{\gamma} \omega_i (K_{2i} - T_{gi} + T)$$

Price Jr. & Romdhane. AIChE J. 2003. 49, 309

Key Diffusivity Parameters

- $D_{0,i}$: infinite-dilution diffusion coefficient
- ξ_{iN}: solvent i to polymer N jumping unit ratio
- $\hat{V}_i^*$: critical hole volume of component i
- K_{1i}/γ: solvent free-volume params.
- $K_{2l} - T_{gl}$: polymer free-volume params.

Key Thermodynamic Parameter

- $\chi_{r,ij}$: FH binary interaction parameter

Parameter Fitting and Single-Solvent System

Measured Residual Solvent

$$r_{i,exp} = \frac{m_{coating}(t_i) - m_{poly}}{A}$$

Predicted Residual Solvent

$$r_{i,pred} = \int_{x=0}^{x=h(t)} c_i(x, t_i) dx$$

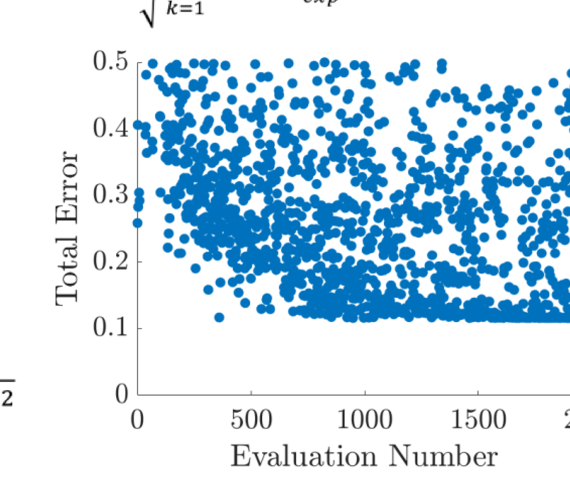
Individual Experimental Error

$$e_1^k = \sum_{j=1}^{N_{pts}} \sqrt{\frac{\left(1 - \frac{r_{i,pred}}{r_{i,exp}}\right)^2}{N_{pts}}}$$

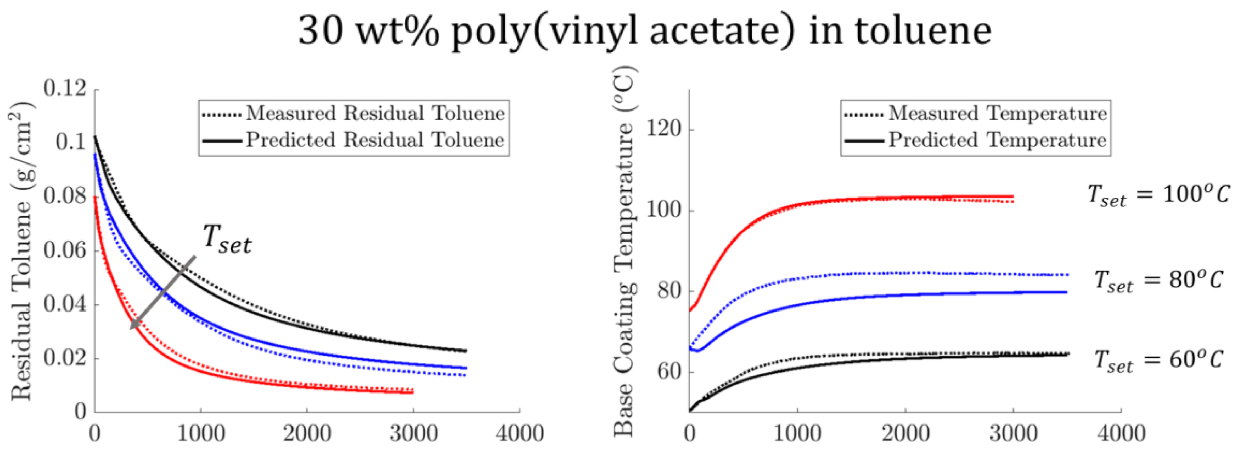
$$e_2^k = \sum_{j=1}^{N_{pts}} \sqrt{\frac{1}{100}\left(\frac{r_{i,exp} - r_{i,pred}}{r_{i,exp}(t_{end}) - r_{i,exp}(0)}\right)^2}$$

Total Regression Error

$$e_{total} = \sqrt{\sum_{k=1}^{N_{exp}} \frac{0.5(e_1^k)^2 + 0.5(e_2^k)^2}{N_{exp} - 1}}$$

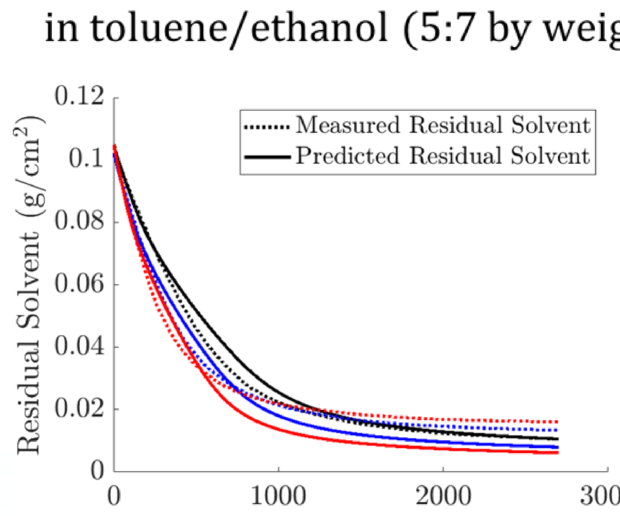


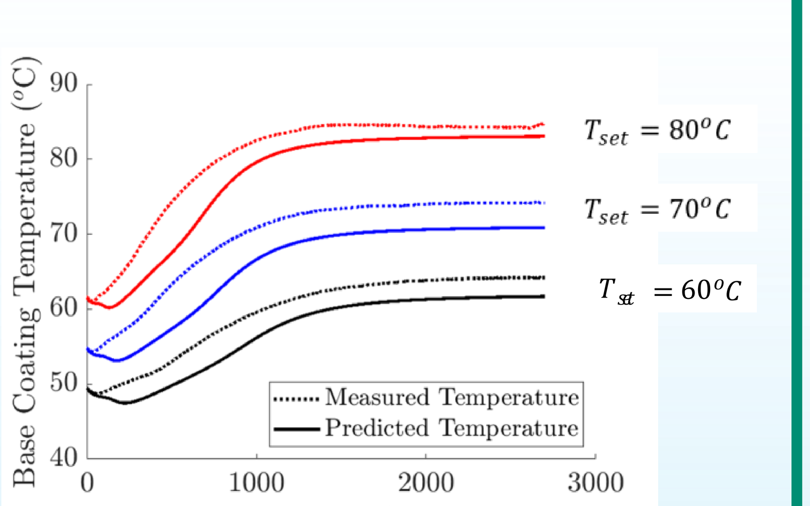
30 wt% poly(vinyl acetate) in toluene



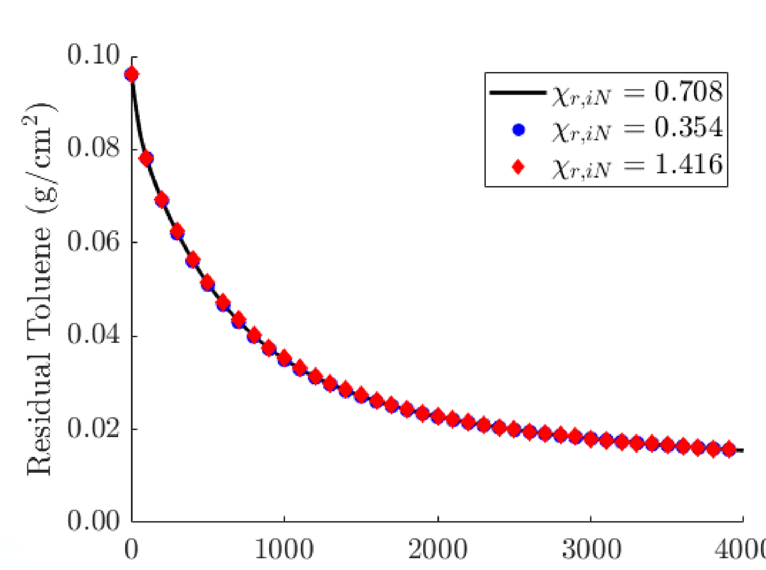
Two-Solvent System

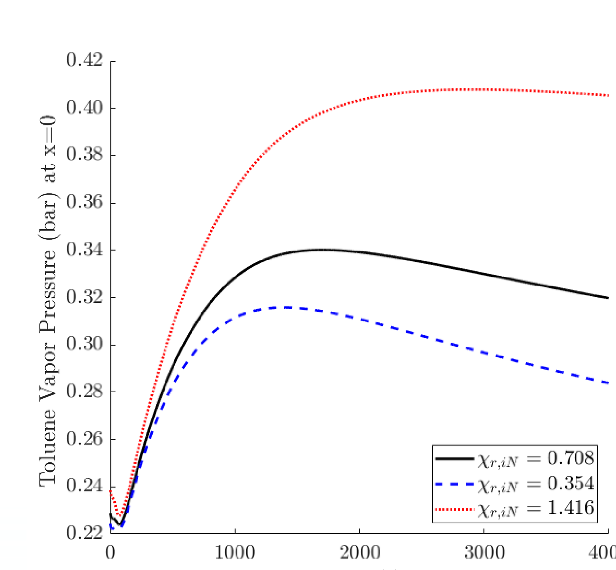
20 wt% poly(vinyl acetate) in toluene/ethanol (5:7 by weight)



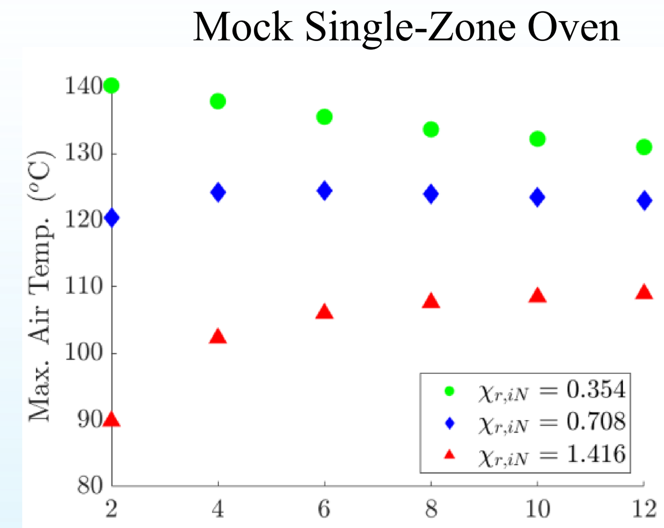


Thermodynamic Parameters and Operating Limits





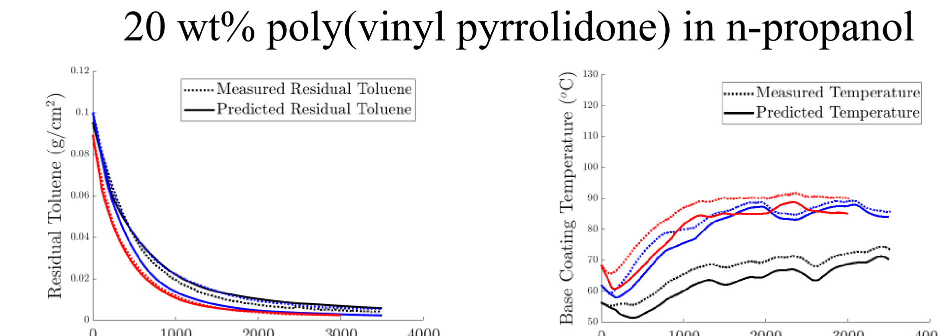
Mock Single-Zone Oven



- Model predictions of residual solvent insensitive to Flory-Huggins interaction parameter
- Representative range of Flory-Huggins parameters yields large variations in vapor pressure (~0.1 bar)
- Variation in vapor pressure yields large spread of maximum operating temperatures for varying Flory -Huggins parameter

Conclusions

20 wt% poly(vinyl pyrrolidone) in n-propanol



- Updated models and regression are needed to account for viscoelastic effects for fast-drying coatings
- Uncertainty in Flory-Huggins Parameter hinders prediction of process operating limits

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