SWELLING OF WOOD. PART IV. A STATISTICAL MODEL FOR PREDICTION OF MAXIMUM SWELLING OF WOOD IN ORGANIC LIQUIDS

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ABSTRACT

A statistical model for prediction of the maximum extent of the swelling of wood in organic liquids is proposed in this work. Solvent basicity, solvent molecular volume, and density of wood appeared to be the most important parameters in the proposed model. The addition of the hydrogen bonding capability parameter did not significantly improve the model.

Keywords: Wood swelling, maximum tangential swelling, solvent basicity, molar volume, hydrogen bonding parameter.

INTRODUCTION

The swelling of wood in organic liquids is of fundamental significance to a wide range of commercial and experimental processes. Wood swelling is a complex process affected by many variables, none of which can individually predict the final maximum extent of the swelling of wood in various organic liquids (Nayer 1948; Stamm 1964; Mantanis et al. 1994a, b, Mantanis 1994). However, statistical analysis allows the assessment of the significance of each of the various parameters on the wood swelling for incorporation into a general regression equation model. The model would then allow prediction of the wood swelling based only on solvent and wood parameters and would be useful for both researchers and practitioners interested in, for example, chemical modification reactions of wood or solvent impregnation processes.

SUMMARY OF PREVIOUS WORK

Nayer (1948) and Stamm (1964) suggested that the best predictor of wood swelling is the hydrogen bonding ability of the swelling solvent. Swelling data gave a reasonably positive correlation; however, there were several significant exceptions to this correlation (di-n-butylamine, tri-n-butylamine, benzaldehyde). Mantanis et al. (1994b) also noted the impor-

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tance of the hydrogen bonding parameter on the wood swelling (maximum tangential swelling) in an extensive series of organic liquids. In addition, Mantanis et al. (1994b) found that solvent basicity (donor number) and molar volume of the swelling liquid were also very significant factors. Wood density also has been found to be an important factor that significantly influences the swelling of wood (Stamm 1935, 1964; Mantanis et al. 1994a). Direct correlations of wood swelling with other properties such as dielectric constant, cohesive energy density, dipole moment, volubility parameter, and surface tension have generally been unsuccessful (Nayer 1948; Stamm 1964; Mantanis et al. 1994b).

METHODS

The most obvious approach to the problem of predicting the extent of wood swelling was a statistical regression analysis of available experimental data (Mantanis et al. 1994b). With this technique, the dependent variable (maximum tangential swelling of wood) was seen as a function of a set of explanatory variables (basicity, molar volume, wood density, hydrogen bonding parameter, molecular weight). The computer-assisted analysis (minitab) then allowed for an analytical evaluation of the relative effect of each of the explanatory variables. This type of analysis provided measures of strength and significance of each association through the resulting regression coefficients and variance effects. The overall percent of variation in the maximum tangential swelling of wood (S) was assessed by the multiple R-square value. Stepwise model-fitting procedures were used to construct the most robust models through evaluation of the various independent variables on the fit. Such models usually have the following basic form:

$$S = \alpha + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \ldots \quad (1)$$

where S = maximum wood swelling, a = constant, x = independent variables and (b_i= partial contribution to swelling of variable xi.

The experimental data utilized for construction of the model were obtained from previous work by the authors (Mantanis et al. 1994a, b). Since a detailed description of the experimental approaches and tabularized data is given in these publications, only a brief description of the experimental procedures is given here.

TABLE 1. *Properties of swelling liquids used in statistical analysis.*

Swelling liquids	Solvent basicity[1] (kcal/mole)	Hydrogen bonding[2] (wave-number shift × 10)	Molar volume[3] (cc)	Molecular weight
Water	18.00	39.00	18.05	18.02
Formamide	24.00	21.50	39.90	45.04
Methanol	19.00	18.70	40.70	32.04
Ethanol	20.00	18.70	58.50	46.07
Propanol	18.00	18.70	75.00	60.10
Dimethylformamide	26.60	11.70	77.00	73.10
Pyridine	33.10	18.10	80.40	79.10
Acetone	17.00	9.70	74.00	58.10
Dioxane	14.80	9.70	85.70	88.10
Ethylacetate	17.10	8.40	98.50	88.10
Methylacetate	16.50	8.40	79.70	74.10
Propylacetate	17.40	8.60	115.70	102.10
Nitromethane	2.70	2.50	54.00	64.10
Chloroform	7.00	1.50	80.70	120.40
Carbon tetracloride	3.00	0.00	97.10	153.80
Nitrobenzene	4.40	2.80	102.30	123.10
Octane	0.00	0.00	162.50	114.20
DMSO	29.80	7.70	71.00	78.10
Acetic	25.00	9.70	57.10	60.00
Butylamine	57.00	16.80	98.80	73.10
Toluene	3.00	4.50	106.40	92.10
Ethylene glycol	18.00	20.60	55.80	62.10

[1] Gutmann 1976.
[2] Crowley et al. 1966; Gordy 1939, 1941.
[3] Robertson 1964; Handbook of Chemistry and Physics 1993.

Dry organic solvents were selected as representatives of various solvent chemical classes. These organic liquids had different properties (hydrogen bonding parameter, molar volume, cohesive energy density, basicity, dipole moment, dielectric constant, volubility parameter, etc.). It is known that these solvent properties influence the wood swelling phenomenon in various ways. Therefore, their selection was chosen in such a way that we were able to determine their relative effect on the swelling of wood.

Heartwood samples of Sitka spruce and

Douglas-fir (softwoods), sugar maple and quaking aspen (hardwoods) were selected for the investigation. These wood species were selected as representative of softwoods and hardwoods with different compositions and densities. Their density varied from 0.4 to 0.7 g/cc, and their extractives contents were very different. The samples were cut in the form of 25-(tangential) x 25-(radial) x 5-(longitudinal) mm pieces and oven-dried for 48 hours at 65 C. Their average moisture content (MC) was 6–7% in the oven-dry basis.

All initial measurements were made at room temperature with a jaw-type vernier caliper, accurate to ±0.05 mm and with jaws sufficient to cover the full 25-mm block side of each wood sample. The oven-dry cross sections were transferred from the oven and cooled in a desiccator. The cooled oven-dry weights and tangential dimensions were measured as quickly as possible. The maximum tangential swelling of the wood blocks in the dry organic liquids was determined in sealed weighing bottles placed in a thermostatically controlled bath (~23 C) for 100 days. The rate of wood swelling in all the organic solvents at room temperature was evaluated using a computerized linear variable displacement transformer (LVDT) apparatus previously described (Mantanis et al. 1994a) with small intervals of time (15-600 sec).

RESULTS AND DISCUSSION

As discussed previously, solvent basicity (donor number), molar volume, wood density, hydrogen bonding capability parameter, and molecular weight were the most important factors influencing the wood swelling phenomena (Mantanis et al. 1994b). The properties of the swelling solvents are shown in Table 1 (donor number data from the literature were available for only twenty-two of the swelling liquids used in our investigation). After statistical analysis, it was found that the best predictive model for the maximum tangential swelling of wood in organic liquids is that which includes three variables–the solvent basicity (SB), the solvent molecular volume (MV), and the density of wood species (WD) (numbers in parentheses are standard deviations).

$$S = \underset{(1.25)}{2.27} + \underset{(0.016)}{0.316}\ SB - \underset{(0.0068)}{0.0426}\ MV + \underset{(1.94)}{4.92}\ WD$$

The R-square value of the regression model was 0.826, and the standard deviation was 2.07%. The typical plot of the residuals versus fitted values showed a reasonable fit. It should also be noted that the addition of the hydrogen bonding parameter into this statistical model did not significantly improve the fit (*R*-square value = 0.828).

CONCLUSIONS

A model based upon a statistical regression analysis of wood swelling experimental data with the basicity and molar volume of the swelling liquid, as well as with the density of wood species. was found to be a good predictor of the maximum tangential swelling of wood.

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