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# Simulation of Drying Nonaqueous Systems—An Application of Simprosys Software

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Drying software, Simprosys (Simprotek Corp., California, USA), for nonaqueous systems is described briefly and applied to a case study. A closed-loop ethanol-nitrogen drying system is modeled with Simprosys 2.1. Simulation results including a parametric evaluation are presented and discussed.

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**Keywords** Dryer design; Drying simulation; Ethanol-nitrogen drying; Psychrometrics; Simprosys

## INTRODUCTION

Drying of materials containing organic solvents or liquids is frequently encountered in the pharmaceutical and fine chemical industries. Based on the flash point of the organic liquid involved, either air or an inert gas can be used as the drying medium. For an organic liquid that has a high flash or burning point, air can be used. However, an inert gas such as nitrogen has to be used for organic liquid of low burning point to prevent possible explosion. In some instances it may be possible to use flue gases with low oxygen content or superheated steam or very high-humidity air to lower oxygen concentration below the flash point of the nonaqueous solvent (or solvent mixture).

A literature search leads to limited effort devoted to drying of nonaqueous systems. Handbooks by Mujumdar<sup>[1]</sup> and Perry<sup>[2]</sup> contain only a few psychrometric charts for nonaqueous systems. With these charts users must use a ruler to measure and read data on the charts and then plug the data into their calculations. It is obviously inadequate for engineers and university students to do their drying calculations this way in this electronic age.

Simprosys, a Windows-based software package, developed by Simprotek Corporation (<http://www.simprotek.com>), provides an integrated, powerful, yet highly user-friendly, contemporary tool for the design and simulation of a dryer

flow sheet as well as drying systems not only for aqueous but for the commonly encountered nonaqueous drying systems. Since the release of its first version for water–air drying systems,<sup>[3]</sup> Simprosys was developed into its advanced version 2.1 to handle 11 additional nonaqueous drying systems. The 11 other nonaqueous drying systems include ethanol–air, ethanol–nitrogen, carbon tetrachloride–air, benzene–air, toluene–air, acetone–nitrogen, methanol–nitrogen, N-propanol–nitrogen, isopropanol–nitrogen, N-butanol–nitrogen, and isobutanol–nitrogen.

For the most common air–water system, Simprosys 2.1 supports 19 unit operations.<sup>[4]</sup> For its other 11 nonaqueous drying systems, Simprosys 2.1 supports 15 unit operations (viz. solids dryer, cyclone, air filter, bag filter, electro-static precipitator, scrubber/condenser, fan/blower, compressor, valve, heater, cooler, heat exchanger, mixer, tee, and pump) and a logical unit operation, recycle.

For information about software or programs applicable to drying, please refer to Gong and Mujumdar,<sup>[4]</sup> Kemp,<sup>[5]</sup> Kemp et al.,<sup>[6]</sup> and Menshatina and Kudra.<sup>[7]</sup> It is worthwhile to mention that a software package called DrySPEC2 (DRYer System for Property and Energy Control), developed by NIZO food research (Ede, The Netherlands), is available for modeling spray dryers.<sup>[8,9]</sup> Another effort worth mentioning is the application of Microsoft Excel combined with Visual Basic used to model and simulate dryer designs.<sup>[10]</sup>

In the following sections a brief introduction is provided for the reader to understand the basic principles and application of this unique software.

## PRINCIPLES OF SIMPROSYS 2.1

For the water–air system, the properties (including saturation pressure) of water are calculated according to the 1967 ASME Steam Tables.

The properties of the organic liquids supported in Simprosys 2.1 are based on Perry<sup>[2]</sup> (section 2, Physical and Chemical Data), Yaws,<sup>[11]</sup> and Yaw and Gabbula.<sup>[12]</sup> The properties of dry air and nitrogen are also based on Perry<sup>[2]</sup> (section 2).

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The drying flow sheet model and dryer model of Simprosys are based on comprehensive studies of the world's most authoritative handbooks by Mujumdar,<sup>[1,13]</sup> Masters,<sup>[14]</sup> and Perry.<sup>[2,15]</sup>

For details about the material property model and other unit operation models in Simprosys, please refer to Gong and Mujumdar.<sup>[4]</sup>

The models for the calculations of absolute humidity, relative humidity, wet-bulb temperature, dew point temperature, humid volume, humid heat, and humid enthalpy are based on the equations in Pakowski and Mujumdar.<sup>[16]</sup>

For a gas–liquid system, the governing equation of wet-bulb temperature is<sup>[16,17]</sup>

$$\frac{t - t_{WB}}{Y - Y_{s,WBT}} = -\frac{\Delta h_{v,WBT}}{c_H} Le^{-2/3} \phi \quad (1)$$

in which  $t$  and  $t_{WB}$  are the dry-bulb and wet-bulb temperatures, respectively;  $Y$  is the absolute humidity;  $Y_{s,WBT}$  is the saturation humidity at wet-bulb temperature;  $\Delta h_{v,WBT}$  is the latent heat of evaporation at wet-bulb temperature;  $c_H$  is the humid heat;  $Le$  and  $\phi$  are Lewis number and humidity potential coefficient defined by

$$Le = \frac{\lambda_g}{c_P \rho_g D_{AB}} \quad (2)$$

and

$$\phi = \frac{M_A/M_B}{Y^* - Y} \ln \left( 1 + \frac{Y^* - Y}{M_A/M_B + Y} \right) \quad (3)$$

in which  $\lambda_g$ ,  $c_P$ , and  $\rho_g$  are the thermal conductivity, specific heat, and density of the humid gas;  $M_A$  and  $M_B$  are the molar mass of the moisture and dry gas;  $Y^*$  is the saturation humidity; and  $D_{AB}$  is the binary diffusivity between the moisture and the gas.

For a water–air system  $Le^{-2/3} \phi \approx 1$  and it is well accepted that  $Le^{-2/3} \phi = 1$ . For carbon tetrachloride–air, benzene–air,

and toluene–air systems, the values of  $Le^{-2/3} \phi$  are from Perry<sup>[2]</sup> (section 12, Psychrometry, Evaporative Cooling, and Solids Drying).

For any other liquid–gas system the values of  $Le^{-2/3} \phi$  are calculated according to Eqs. (2) and (3). The value of  $D_{AB}$  in Eq. (2) is based on Fuller et al.<sup>[18,19]</sup> and Poling et al.<sup>[20]</sup>

$$D_{AB} = \frac{0.01013 T^{1.75} \left( \frac{1}{M_A} + \frac{1}{M_B} \right)^{\frac{1}{2}}}{P [(\sum A v_i)^{\frac{1}{3}} + (\sum B v_i)^{\frac{1}{3}}]^2} \quad (4)$$

in which  $T$  and  $P$  are the temperature and pressure of the liquid–gas system. Units of  $T$  and  $P$  are K and Pa, respectively, with the resulting diffusivity in  $m^2/s$ . All  $v_i$  are group contribution values for the subscript component summed over atoms, groups, and structural features given in table 3 of Fuller et al.<sup>[19]</sup> or tables 11-1 of Poling et al.<sup>[20]</sup>

Please note that Eqs. (2)–(152) in Perry<sup>[2]</sup> cited from Fuller et al.<sup>[19]</sup> has a wrong coefficient of 0.10103, which should be 0.01013.

## A CLOSED-LOOP ETHANOL–NITROGEN SYSTEM

Drying of materials containing nonaqueous solvents is generally carried out in a closed-loop system so that the exhaust gas containing nonaqueous vapors is not discharged into the atmosphere to pollute the air.

Simprosys 2.1 is applied to the drying of a solid material containing ethanol. Due to the low flash (burning) point, nitrogen is used as the drying gas to prevent possible explosion hazard. In order to avoid losing both the ethanol and the nitrogen drying gas in the exhaust, a closed-loop drying system as displayed in Fig. 1 is needed.

The input and output conditions of the drying material and nitrogen drying gas are as follows: material feed temperature = 20°C; feed moisture content = 0.08 kg/kg wet basis; wet material mass flow rate = 2000 kg/h; product temperature = 50°C; product moisture content = 0.002 kg/kg wet basis; nitrogen pressure at dryer inlet = 102.4 kPa;

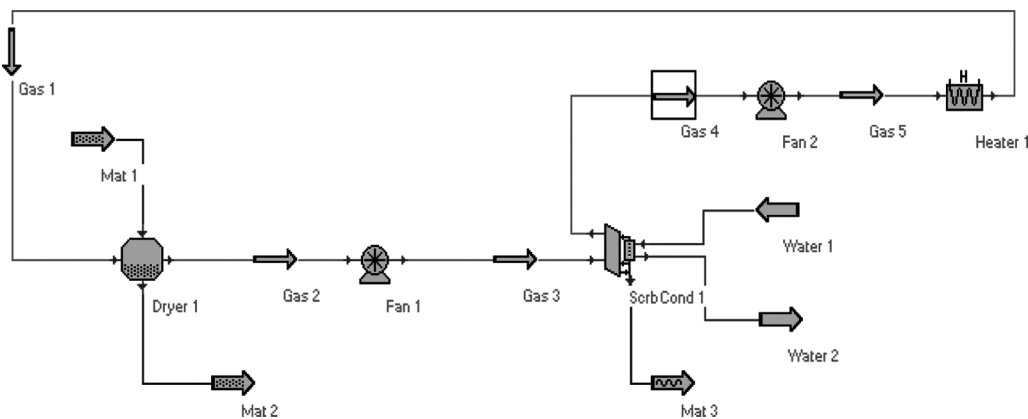


FIG. 1. Flow sheet of a closed-loop nitrogen–ethanol system.

temperature at dryer inlet = 120°C; mass flow rate wet basis at dryer inlet = 3000 kg/h.

The pressure drop in the dryer is 1.2 kPa. The dryer gas outlet stream goes through a fan to gain 1.5 kPa static pressure. The efficiency of the fan is 0.75. Exhaust air coming from the fan goes through a scrubber/condenser to collect the dusts and remove the moisture carried in the exhaust air. The temperature of the exhaust air from the scrubber/condenser is 35°C. The air pressure drop in the scrubber/condenser is 1.0 kPa. The collection efficiency and liquid-gas ratio of the scrubber/condenser are 99% and 1.0, respectively. The liquid inlet pressure and temperature of the scrubber/condenser are 101.3 kPa and 20°C. The air coming out of the scrubber/condenser goes through a fan to gain some static pressure and then goes through a heater to be heated to the required dryer inlet temperature (120°C). The efficiency of the fan is set at 0.75. The pressure drop of air in the heater is 0.6 kPa.

The flow sheet is constructed as shown in Fig. 1. The simulation results produced using Simprosys 2.1 are displayed in Fig. 2.

Please note that one can use the heating duty of the heater instead of the dry-bulb temperature of the dryer gas inlet and/or the dry-bulb temperature of the dryer gas outlet instead of the moisture content of the material inlet as input parameter to simulate the operation of an existing drying system.

Parametric studies are carried out to investigate the effects of several major operational parameters on other process parameters such as scrubber/condenser cooling duty, heater heating duty, and dryer exhaust gas temperature and relative humidity.

### Effects of Scrubber/Condenser Gas Outlet Temperature

All input parameter values are kept the same in the flow sheet (Fig. 2) except for changing scrubber/condenser gas outlet temperature to see how it affects other process parameters. The simulation results are displayed in Table 1.

From Table 1 one can see that with an increase of the scrubber/condenser gas outlet temperature, both the scrubber/condenser cooling duty and the heater heating duty decrease, but the dryer exhaust gas relative humidity and temperature increase.

When the scrubber/condenser gas outlet temperature is increased, the saturation moisture content of the gas increases. This leads to increased dryer gas inlet moisture content. Increased gas moisture content results in decreased mass transfer for the dryer, which means an increased dryer size for a design, which means increased equipment cost. Therefore, for the same evaporation duty in the design of such a closed-loop drying system, a larger dryer is required if a higher scrubber/condenser gas outlet temperature is adopted, with the consequence of increased equipment cost but decreased operating cost due to less

Edit Flowsheet Data										
Close Report Customize...										
Gas Streams:					Scrubber Condensers:					
	Gas 1	Gas 2	Gas 3	Gas 4	Gas 5	ScrbCond 1				
Mass Flow Rate Wet Basis (kg/h)	3000.000	3156.313	3156.313	3000.000	3000.000	Gas Pressure Drop (kPa)	1.000			
Mass Flow Rate Dry Basis (kg/h)	2382.808	2382.808	2382.808	2382.808	2382.808	Collection Efficiency	0.990			
Volume Flow Rate (m <sup>3</sup> /h)	3140.019	2727.055	2696.414	2478.079	2454.358	Inlet Particle Loading (g/m <sup>3</sup> )	0.000			
Pressure (kPa)	102.400	101.200	102.700	101.700	103.000	Outlet Particle Loading (g/m <sup>3</sup> )	0.000			
Dry-bulb Temperature (°C)	120.000	53.052	54.167	35.000	35.952	Particle Collection Rate (kg/h)	0.000			
Wet-bulb Temperature (°C)	78.678	39.953	40.318	35.000	35.320	Particle Loss to Gas Outlet (kg/h)	0.000			
Dew Point Temperature (°C)	35.128	38.534	38.817	35.000	35.237	Cooling Duty (kW)	62.010			
Absolute Humidity (kg/kg)	0.259	0.325	0.325	0.259	0.259	Liquid Gas Ratio	1.000			
Relative Humidity	0.033	0.488	0.470	1.000	0.963	Liquid Recirc. Mass Flow (kg/h)				
Specific Enthalpy (kJ/kg)	331.146	290.803	292.065	232.871	233.920	Liquid Recirc. Volume Flow (m <sup>3</sup> /h)	2696.414			
Humid Heat (kJ/kg.°C)	1.497	1.532	1.533	1.415	1.416	Dryers:		Dryer 1		
Density (kg/m <sup>3</sup> )	0.955	1.157	1.171	1.211	1.222	Gas Pressure Drop (kPa)	1.200			
Material Streams:										
	Mat 1	Mat 2	Mat 3							
Mass Flow Rate Wet Basis (kg/h)	2000.000	1843.687	156.313							
Mass Flow Rate Dry Basis (kg/h)	1840.000	1840.000								
Volume Flow Rate (m <sup>3</sup> /h)			0.198							
Pressure (kPa)			101.300							
Temperature (°C)	20.000	50.000	20.000							
Vapor Fraction			0.000							
Moisture Content Wet Basis (kg/kg)	0.080	0.002	1.000							
Moisture Content Dry Basis (kg/kg)	0.087	0.002								
Mass Concentration (kg/kg)			0.000							
Specific Enthalpy (kJ/kg)	26.900	63.119	46.455							
Specific Heat (kJ/kg.°C)	1.351	1.263	2.398							
Specific Heat Dry Basis (kJ/kg.°C)	1.468	1.265								
Density (kg/m <sup>3</sup> )			790.357							
						Fans:		Fan 1 Fan 2		
						Static Pressure (kPa)	1.500	1.300		
						Total Discharge Pressure (kPa)	1.500	1.300		
						Efficiency	0.750	0.750		
						Power Input (kW)	1.515	1.193		
						Heaters:		Heater 1		
						Heating Duty (kW)	81.021			
						Pressure Drop (kPa)	0.600			

FIG. 2. Simulation results of the nitrogen-ethanol system.

TABLE 1  
Effects of scrubber/condenser gas outlet temperature

Scrubber/condenser gas outlet temperature (°C)	Scrubber/condenser cooling duty (kW)	Heater heating duty (kW)	Dryer gas outlet temperature (°C)	Dryer exhaust gas relative humidity
25	69.03	86.82	51.33	0.345
35	62.01	81.02	53.05	0.488
45	55.27	75.86	55.40	0.676

energy consumption. To the contrary, a smaller dryer is required if a lower scrubber/condenser gas outlet temperature is adopted, which means lower equipment cost but increased operating cost due to higher energy consumption.

### Effects of Material Inlet Moisture Content

All input parameter values (including the material outlet moisture content wet basis, 0.002) are kept the same in the flow sheet (Fig. 2) except for changing the material inlet moisture content to see how it affects other process parameters. The simulation results are displayed in Table 2.

From Table 2 one can see that with an increase of the material inlet moisture content, the scrubber/condenser cooling duty and the heater heating duty stay about the same; the dryer exhaust gas relative humidity increases, but the dryer exhaust gas temperature decreases.

With an increase in the material inlet moisture content the evaporation duty increases because the specified material outlet moisture content stays the same. This results in more heat to be spent to evaporate the increased ethanol liquid. Therefore, the dryer gas outlet temperature

decreases, which results in the increase of the dryer gas outlet relative humidity.

One may expect the scrubber/condenser cooling duty and the heater heating duty to increase due to the increased material inlet moisture content. Because no extra heat is added into the system in spite of the increased evaporation duty, this results in a decrease of the dryer gas outlet temperature.

If the drying kinetics (which are to be developed in the future version of Simprosys) are taken into consideration for an existing system, when there is an increase in the material inlet moisture content, the dryer gas inlet temperature has to be increased to increase the heat and mass transfer to satisfy the material outlet moisture content requirement. In that case, the scrubber/condenser cooling duty and the heater heating duty will have to increase to balance the increases heat input in the system.

### Effects of Dryer Gas Inlet Temperature

All input parameter values are kept the same in the flow sheet (Fig. 2) except for changing the dryer gas inlet temperature to see how it affects other process parameters. The simulation results are displayed in Table 3.

TABLE 2  
Effects of material inlet moisture content

Material inlet moisture content (kg/kg wet basis)	Scrubber/condenser cooling duty (kW)	Heater heating duty (kW)	Dryer gas outlet temperature (°C)	Dryer gas outlet relative humidity
0.07	61.81	81.02	58.42	0.373
0.08	62.01	81.02	53.05	0.488
0.09	62.23	81.02	47.77	0.641

TABLE 3  
Effects of dryer gas inlet temperature

Dryer gas inlet temperature (°C)	Scrubber/condenser cooling duty (kW)	Heater heating duty (kW)	Dryer gas outlet temperature (°C)	Dryer exhaust gas relative humidity
110	52.50	71.15	43.67	0.769
120	62.01	81.02	53.05	0.488
130	71.59	90.96	62.44	0.318

From Table 3, one can see, as is expected, with an increase of the dryer gas inlet temperature, the scrubber/condenser cooling duty, the heater heating duty, and the dryer gas outlet temperature increase, but the dryer exhaust gas relative humidity decreases due to the increased dryer gas outlet temperature.

### CLOSING REMARKS

Simprosys provides an integrated, powerful, highly user-friendly, contemporary, but cost-effective tool for the design and simulation of dryer and drying systems involving not only aqueous systems but 11 commonly encountered nonaqueous systems. Extension of Simprosys 2.1 to other nonaqueous systems is simple and easy on demand.

Simprosys makes tedious complicated thermal calculations simple for the design and simulation of dryers and drying systems. Typical calculations of a process that may take one skilled engineer weeks to carry out can now be accomplished in hours with Simprosys. This software can be used to examine (optimize and/or troubleshoot) existing drying systems, modifying existing systems, and evaluate new systems before they are installed.

Simprosys has intuitive user interfaces with maximum protection to prevent users from making simple mistakes. It also has an effective tutorial to teach users step by step how to use the software to simulate typical drying- and evaporation-related systems. Users of Simprosys will require minimal self-training and effort to use it effectively.

Interested readers may visit <http://www.simprotek.com> to download a free trial version to explore the capability of Simprosys for their own applications.

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