Description of process

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1 Introduction

Crystallization occurs in single-effect evaporators, commonly known as vacuum pans. Figure 1 shows a schematic of a vacuum pan, highlighting the input and output flows to the system. The pan is initially filled up to 50% of its capacity with a sucrose solution called magma, which contains water, impurities, crystals, and dissolved sucrose. Following this, a feed flow F_f is introduced, which includes water, sucrose, and impurities. Heating Steam F_{hs} is then applied to the pan's calandria, all the heating steam applied is condensed as water F_{cw}. The calandria is a separate chamber, preventing the steam from mixing with the magma. As the steam is applied, the water in the pan evaporates $\dot{m}_{vap}$.

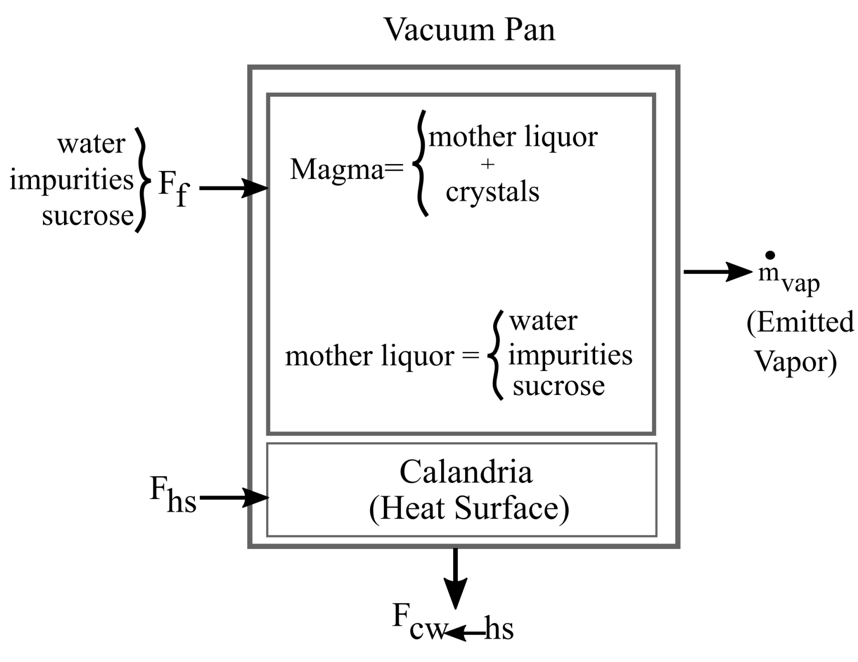

Figure 1: Vacuum Pan.

2 Description of Data

Figure 2 shows the input and output variables measured in the process, which correspond to the available historical data. In total, data from 7 batches are available, attached in the .mat files. The data were recorded with a sampling time of 10 seconds.

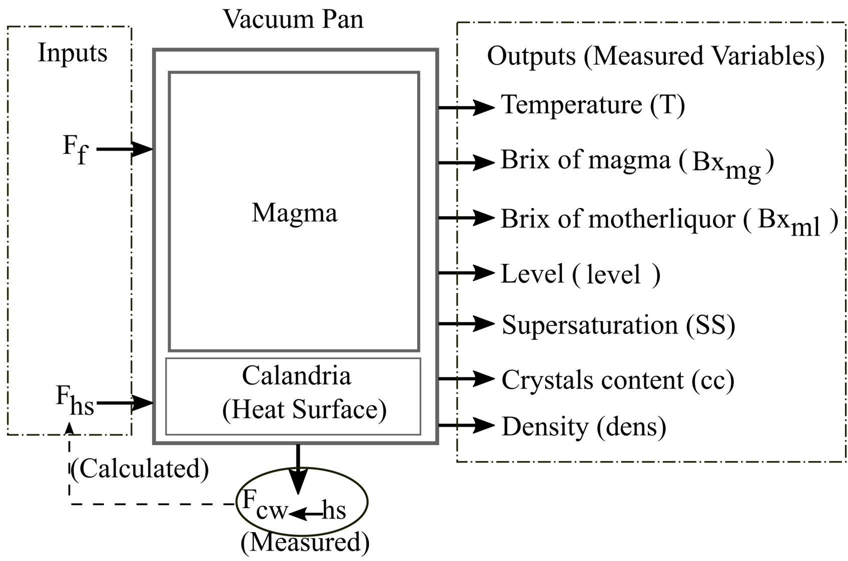

Figure 2: Vacuum Pan.

2.1 Data:

The following table shows a description of the measured input and output variables, the calculated variables, and the states of the model. The variables described in the table are part of the .mat data files attached.

	Measured Variables
T	Temperature (°C)
N	Mass Level (%)
Bx_{ml}	Brix of mother liquor (°bx)
Bx_{mg}	Brix of magma (°bx)
SS	Supersaturation
CC	Crystal content (%)
$dens$	Mass density (kg/m^3)
F_{cw}	Condensate water (m^3/s)
	Other Measured Variables (Not Used in the Model)
T_{vapor}	Heating steam temperature (°C)
$Vacio$	Vacuum pressure inside crystallizer (inHg) (Considered constant in the model)
$Viscd$	Mass viscosity
	Inputs
F_{hs}	Condensate water from heating steam (m^3/s) (Calculeated from F_{cw}), see Eq 9
F_f	Feed flow rate (m^3/s)
	Calculated Variables (Considered as Real Data)
Model States	
M_w	Mass of water (kg)
M_i	Mass of impurities (kg)
M_c	Mass of crystals (kg)
M_s	Mass of dissolved sucrose (kg)
T	Temperature (Temperature is directly measured)
Purities	
P_{mg}	Purity of magma
P_{ml}	Purity of mother liquor

Table 1: Measured Variables, Inputs, and Calculated Variables

2.2 Description of the attached files:

- Simulation.mat: File for simulating the model. This file simulates the crystallization model described below, applying real inputs and comparing its output with actual process data (The model is simulated in discrete time).
- data.mat: Contains historical data for the 7 available batches.

3 Model description

Crystallization processes are usually described through mass, energy, and crystal population balances. In this case, the third stage of crystallization is modeled. The modeling leads to a set of five ordinary differential equations (ODEs). The extended structure of the model is completed with kinetic expressions, phase equilibrium relationships, and correlations necessary to determine the physical properties of the substances, as well as the relevant relationships to describe the heat and mass transfer phenomena in the process.

Water Balance:

$$\frac{\mathrm{d}m_w(t)}{\mathrm{d}t} = \rho_f F_f(t)\left(1 - \frac{B_f^{\%}}{100}\right) - \dot{m}_{vap}(t) \tag{1}$$

Impurities Balance:

$$\frac{\mathrm{d}m_i(t)}{\mathrm{d}t} = \rho_f F_f(t)\frac{B_f^{\%}}{100}\left(1 - \frac{P_f^{\%}}{100}\right) \tag{2}$$

Crystals Balance:

$$\frac{\mathrm{d}m_c(t)}{\mathrm{d}t} = cc(t)\left(\rho_f F_f(t) - \dot{m}_{vap}(t)\right) + \alpha_c \tag{3}$$

Sucrose balance:

$$\frac{\mathrm{d}m_s(t)}{\mathrm{d}t} = \rho_f F_f(t)\frac{B_f^{\%}}{100}\frac{P_f^{\%}}{100} - \frac{\mathrm{d}m_c(t)}{\mathrm{d}t} \tag{4}$$

Energy Balance:

$$\frac{\mathrm{d}T_{mg}(t)}{\mathrm{d}t} = \frac{W + Q_{hs} + \rho_f F_f(t)\left(h_f - h_{ml}\right) - \dot{m}_{vap}(t)L_{vap} + J_c(t)L_c}{\left[m_w(t) + m_i(t) + m_c(t) + m_s(t)\right]Cp_{mg}} \tag{5}$$

with

$$cc(t) = \frac{m_c(t)}{m_w(t) + m_i(t) + m_c(t) + m_s(t)} \tag{6}$$

$$\dot{m}_{vap}(t) = \rho_{cw}\alpha_{vap}\alpha_q^{-1}F_{hs}(t) \tag{7}$$

$$Q_{hs} = \rho_{cw}\alpha_q^{-1}F_{hs}(t)L_{cw} \tag{8}$$

where

$$F_{hs}(t) = \alpha_q F_{cw\leftarrow hs}(t) \tag{9}$$

$$F_{vap}(t) = \alpha_{vap}F_{cw\leftarrow hs}(t) \tag{10}$$

Nomenclature

m_w	mass of water (kg)
m_i	mass of impurities (kg)
m_c	mass of crystals (kg)
m_s	mass of sucrose (kg)
T_{mg}	magma temperature (°C)
ρ_f	density of the feed volumetric flow (kg/m^3)
F_f	feed volumetric flow (m^3/s)
$B_f^{\%}$	brix of the feed flow (°bx)
cc	crystal content
$P_f^{\%}$	purity of the feed volumetric flow (%)
$\dot{m}_{vap}$	mass flow of emitted vapor (kg/s)
J_c	crystallization rate (kg/s)
W	power of the electric stirring motor (kW)
Q_{hs}	heat supplied by the heating steam (J/s)
h	specific enthalpy (J/kg)
L	specific latent heat (J/kg)
Cp_{mg}	specific heat capacity $(J/(kg$°C$))$

Subscripts

w	water
i	impurities
c	crystals
s	sucrose
f	feed
cw	condensed water
mg	magma or massecuite
ml	mother liquor

3.1 Correlations for Physical and Thermodynamic Properties

Mass fraction of solids

$$B_{ml} = \frac{m_i + m_s}{m_w + m_i + m_s} \tag{11}$$

$$B_{mg} = \frac{m_i + m_c + m_s}{m_w + m_i + m_c + m_s} \tag{12}$$

Percentage of dissolved solids (°Bx)

$$B_{ml}^{\%} = B_{ml} \times 100 \tag{13}$$

$$B_{mg}^{\%} = B_{mg} \times 100 \tag{14}$$

Mass fraction of sugar

$$P_{ml} = \frac{m_s}{m_i + m_s} \tag{15}$$

$$P_{mg} = \frac{m_c + m_s}{m_i + m_c + m_s} \tag{16}$$

Purity (%)

$$P_{ml}^{\%} = P_{ml} \times 100 \tag{17}$$

$$P_{mg}^{\%} = P_{mg} \times 100 \tag{18}$$

Density (kg/m^3)

$$\rho_f = \left(1000 + \frac{B_f^{\%}\left(200 + B_f^{\%}\right)}{54}\right)\left(1 - 0.036\frac{T_f - 20}{160 - T_f}\right) - 1000\left(1 - e^{\left(1-\frac{P_f^{\%}}{100}\right)\left(1.164\times10^{-4}B_f^{\%}+6.927\times10^{-6}B_f^{\%2}\right)}\right) \tag{19}$$

$$\rho_{mg} = \left(1000 + \frac{B_{mg}^{\%}\left(200 + B_{mg}^{\%}\right)}{54}\right)\left(1 - 0.036\frac{T_f - 20}{160 - T_f}\right) - 1000\left(1 - e^{(1-P_{mg})\left(1.164\times10^{-4}B_{mg}^{\%}+6.927\times10^{-6}B_{mg}^{\%2}\right)}\right) \tag{20}$$

$$\rho_{cw} = 1016.7 - 0.57T_w \tag{21}$$

Specific heat capacity $(J/(kg{\cdot}^{\circ}\mathrm{C}))$

$$Cp_{mg} = 4187 - 29.309B_{mg}^{\%} \tag{22}$$

$$Cp_c = 1163.2 - 3.488T_{mg} \tag{23}$$

$$Cp_{ml} = 4186.8 - 29.7B_{ml}^{\%} + 4.61B_{ml}^{\%}P_{ml} + 0.075B_{ml}^{\%}T_{mg} \tag{24}$$

$$Cp_f = 4186.8 - 29.7B_f^{\%} + 4.61B_f^{\%}\frac{P_f^{\%}}{100} + 0.075B_f^{\%}T_f \tag{25}$$

Specific enthalpy (J/kg)

$$h_f = Cp_fT_f \tag{26}$$

$$h_{ml} = Cp_{ml}T_{mg} \tag{27}$$

$$h_c = Cp_cT_{mg} \tag{28}$$

$$h_w = 2323.3 + 4106.7T_w \tag{29}$$

$$h_{vap} = 2499980 - 24186p_{vac} + (1891.1 + 106.1p_{vac})T_{vap} \tag{30}$$

Specific latent heat (J/kg)

$$L_c = h_{ml} - h_c \tag{31}$$

$$L_{vap} = h_{vap} - h_w \tag{32}$$

$$L_{cw} = 2323.3 + 4106.7T_w + 0.6T_w^2 \tag{33}$$

References