Agrotrópica 1(3): 204 - 212.1989
Centro de Pesquisas do Cacau, Ilhéus, Bahia, Brasil

A MODEL TO SIMULATE THE HEAT AND MOISTURE TRANSFER IN CACAO TRANSPORTED IN CONTAINERS

Ricardo B. Sgrillo[1], *Kátia R. P. Araújo*[2] *and Luiz C. E. Milde*[1]

Centro de Pesquisas do Cacau (CEPEC), CEPLAC, 45600, Itabuna, Bahia, Brasil. [2]Estagiária.

Abstract

A compartmental deterministic model to simulate the heat and moisture transfer in a composite system of cacao beans being delivered in a container inside a ship hold was developed. The model forecasts the temperatures and humidity levels for each component of the system (cacao beans, walls of the container and interior air), as a function of the external temperature (conventional container) and external relative humidity (ventilated container). Comparing the simulated with actual results , there are indications that the model provides a good prediction of the temperatures of each component and also predicts the general tendency of the variations of the moisture levels of each component.

Key words: *Theobroma cacao,* simulation, mathematical model, container.

Modelo para simular as trocas de calor e umidade no transporte de cacau em contentores

Resumo

Desenvolveu-se um modelo determinístico compartimental para simular as trocas de calor e umidade em um sistema composto de amêndoas de cacau transportadas em um contentor no porão de um navio. O modelo prediz as temperaturas e umidades para cada componente do sistema (cacau, paredes do contentor e ar interior), como função das temperaturas externas (contentor convencional) e umidades externas (contentor ventilado). As comparações dos resultados simulados com os reais indicam que o modelo fornece boas predições das temperaturas de cada componente e da tendência geral das variações da umidade nos componentes.

Palavras-chave: *Theobroma cacao,* simulação, modelo matemático, contentor

1. Introduction

Shipment of tropical commodities in containers has shown advantages due to cost reduction and safety increase when compared with conventional transportation forms.

Some products as coffee, cacao and copra, when delivered in containers, have arrived damaged to their destination, because of moisture condensation in cold weather. Sharp and Greve (1984) demonstrated that when these products are delivered from the southern hemisphere, during summer, to the north hemisphere

Received for publication December 5, 1989

the temperature decrease during the trip induces moisture condensation on the ceiling and walls of the containers. Depending on certain conditions water can drop on the product (rainfall effect) resulting in dampening and rotting.

This problem has made cacao transportation in containers from Brazil to be incipient. According to Serôdio and Iturbe (1988) only 4 to 5% of cacao beans is exported in this way from the port of Ilhéus (Bahia, Brazil).

To understand the physical processes which occur inside a container delivering cacao, and looking for possible solutions to the noted problems, a compartmental deterministic mathematical model to simulate the heat and moisture transfer inside a container was developed.

2. The model

The model was developed considering a system formed of a container loaded with jute bags of dry cacacao beans delivered in the hold of a ship.

This system was divided in parts, all of them considered homogeneous, i.e., inside the component there being no important thermal or moistures gradients. The components are:

- ae = external air;
- p = walls and ceiling of container;
- ah = air space between ceilling and top of upper layer of cacao ('head space'- 50 cm);
- ct = upper layer of cacao beans (30 cm width);
- at = interstitial air in the upper layer;
- cp = peripheric layer of cacao beans in contact with the walls and the floor of the container (30 cm width);
- ap = interstitial air of the peripheric layer;
- cc = cacao beans forming the central layer of the container;
- ac = interstitial air at the central layer.

The model basically consists of two systems of differential equations, one representing the heat exchange and another representing the moisture exchange.

The terms units, and parameters of the following equations, are defined in Annex 1.

2.1. Thermal balance

Equation 1 represents the thermal balance at the head space. The heat exchanges of this component are made with the external environment, through the ventilation (in the case of ventilated containers); with the walls and ceilling; with the cacao beans and the interstitial air of the upper layer.

$$Ca * Vah * dTah/dt = Qvent - Qah.p - Qah.ct - Qah.at \quad (1)$$

The thermal balance of the interstitial air of the upper layer is represented by Equation 2. In this case the exchanges are made with the head space air; with the cacao beans of the upper layer; with the interstitial air of the central layer.

$$Ca * Vat * dTat/dt = Qah.at - Qat.ct - Qat.ac \quad (2)$$

Equation 3 represents the thermal balance of the interstitial air of the central layer. The heat exchanges occur with the interstitial air of the upper and peripheric layer and with the cacao beans of the central layer.

$$Ca * Vac * dTac/dt = Qat.ac - Qac.cc - Qac.ap \quad (3)$$

The heat balance in the interstitial air of the peripheric layer, represented by Equation 4, occurs through the heat exchange with the external environment (ventilation); with the interstitial air of the central layer; with the cacao beans of the peripheric layer and with the walls of the container.

$$Ca * Vap * dTap/dt = QVent + Qac.ap - Qap.cp - Qap.p \quad (4)$$

Equation 5 represents the thermal balance in the cacao of the upper layer. In this component, the heat is exchanged with the head air; with the interstitial air of the upper layer; with the cacao beans of the central layer. The heat loss that occurs due to the water evaporation process in the cacao beans of this layer is also considered.

$$Cc * Pct * dTct/dt = Qah.ct + Qat.ct - Qct.cc - Qevct \quad (5)$$

The heat balance of the cacao beans in the central layer is represented by Equation 6. There are heat exchanges between cacao beans of the upper and central layer and the interstitial air of the central layer.

$$Cc * Pcc * dTcc/dt = Qct.cc + Qac.cc - Qcc.cp \quad (6)$$

The specific heat of cacao (Cc) is a function of its content of moisture, being estimated by Equation 6a (data from Almeida, 1979).

$$Cc = SQR\ (8.25E06 + 1.04E06 * Ln\ (Wc/(Wc + 1))) \quad (6a)$$

Equation 7 represents the thermal balance in the cacao beans of the peripheric layer. Heat exchanges occur between the cacao beans of the central layer; the interstitial air of the peripheric layer and with the walls of the container.

$$Cp * Pcp * dTcp/dt = Qcc.cp + Qap.cp - Qcp.p \quad (7)$$

The thermal balance in the walls is represented by Equation 8. There are heat exchanges between the external environment; with the interstitial air and the cacao beans of the upper layer; and with the headspace air. The heat losses and gains increase due to the process of condensation and evaporation of water on the walls, and the exchanges that occur with the external environment by radiation were also considered.

$$Cp * Pp * dTp/dt = Qae.p + Qat.p + Qcond + Qah.p - Qp.ct - Qevpp - Qrad \quad (8)$$

2.1.1. Heat flow

The heat flow by convection between cacao and interstitial air of the different layers, walls, and air, in the head space, and exterior (Qae.p, Qah.at, Qah.ct, Qah.p, Qac.ap, Qac.cc, Qap.cp, Qap.p, Qat.ac, Qat.ct, Qcc.cp, Qcp.p, Qct.cc) were calculated using equations similar to Equation 9 (Kreith, 1977):

$$Qi.j = S'i.j * hi.j * (Ti - Tj) \quad (9)$$

The surfaces of heat exchange between the interstitial air of two layers in contact (equation 9) is calculated by Equation 9a:

$$S'i.j. = Si.j * Po \quad (9a)$$

The coefficients of heat transmission by convection were estimated using a methodology presented by Kreith(1977). With the calibration of the parameters of the model, the following expressions were obtained:

hac.cc	=	1.88	*	(Tac - Tcc)	(10)
hae.p	=	1.36	*	(Tae - Tp)	(11)
hah.at	=	1.88	*	(Tah - Tat)	(12)
hah.ct	=	1.88	*	(Tah - Tct)	(13)
hah.p	=	1.88	*	(Tah - Tp)	(14)
hap.ac	=	0.02	*	(Tap - Tac)	(15)
hap.cp	=	1.88	*	(Tap - Tcp)	(16)
hap.p	=	1.88	*	(Tap - Tp)	(17)
hat.ac	=	0.02	*	(Tat - Tac)	(18)
hat.ct	=	1.88	*	(Tat - Tct)	(19)
hcp.cc	=	0.55	*	(Tcp - Tcc)	(20)
hp.cp	=	1.88	*	(Tp - Tcp)	(21)
hct.cc	=	0.15	*	(Tct - Tcc)	(22)

Heat flow by condensation and evaporation is calculated by Equations 23, 24 and 25 (Arinze, Schoenau and Besant, 1984):

$$Qcond = L * Mcond \quad (23)$$

$$Qevct = L * Mevct \quad (24)$$

$$Qevpp = L * Mevpp \quad (25)$$

In the above equations, L represents the latent heat of water vaporization calculated at temperature T of the component where the process occurs according to Equation 26:

$$L = 3.16E06 - 2.41E03 * T \quad (26)$$

The heat exchange by radiation, between the walls of the container and the walls of the ship hold, are calculated according to Henderson and Perry (1976), using Equation 27:

$$Qrad = Sep * E * SB * (Tpp^4 - Tp^4) \quad (27)$$

Heat exchanges associated with container ventilation are calculated by equation 28 (Sharp and Greve, 1984):

$$Qvent = Vent * Da * Ca * (Tae - Ti) \quad (28)$$

In this equation Vent represents the ventilation rate (m^3/s), calculated according to Equation 29:

$$Vent = J * SQR (1/Tae - 1/Ti) \quad (29)$$

Where J is as a constant calculated according to the ventilator window geometry and dimensions (Sharp and Greve, 1984).

2.2. Water balance

Equation 30 represents the water balance of the air at the head space. Water increases in this component are due to the evaporation of water condensed on the walls and the water in the cacao of the upper layer; the losses are due to condensation on the walls and water absorption by cacao beans. There are humidity exchanges with the external environment, through ventilation, and with the interstitial air of the upper layer.

$$Da * Vah * dWah/dt = Mevpp + Mct.ah + Mvent - Mabsct - Mah.at - Mcond \quad (30)$$

The humidity balance of the interstitial air of the upper layer is due to the exchanges between the cacao beans of this layer, and the headspace and with the interstitial air of the central layer (Equation 31).

$$Da * Vat * dWat/dt = Mct.at + Mah.at - Mat.ac \quad (31)$$

Equation 32 represents the water balance in the interstitial air of the central layer. In this case the exchanges are between the cacao beans of this layer and the interstitial air from the upper and peripheric layers.

$$Da * Vac * dWac/dt = Mcc.ac + Mat.ac + Map.ac \quad (32)$$

The water exchanges that occur in the interstitial air of the peripheric layer are between the cacao beans in this layer; the external environment by ventilation and the interstitial air in the central layer (Equation 33).

$$Da * Vap * dWap/dt = Mcp.ap + Mvent - Map.ac \quad (33)$$

Equation 34 represents the humidity balance of cacao beans in the upper layer. There are gains in the content of water in the air at the head space by absorption, loss of water to the head space air by evaporation and exchanges with the interstitial air of this layer and with the cacao beans of the central layer.

$$Dc * Vct * dWct/dt = Mabsct - Mct.at - Mct.cc - Mct.ah \quad (34)$$

Equation 35 represents the humidity balance in the cacao beans of the peripheric layer. The exchanges, in this case, occur between the interstitial air in this layer and the cacao beans of the upper layer.

$$Dc * Vcp * dWcp/dt = - Mcp.ap - Mcp.cc \quad (35)$$

Equation 36 represents the water balance in the cacao of the central layer. There is water exchange between the interstitial air in this layer and the cacao beans from the upper and peripheric layers.

$$Dc * Vcp * dWcc/dt = Mct.cc + Mcp.cc - Mcc.ac \quad (36)$$

The water balance in the walls and ceiling is represented by Equation 37. There is an increase of water by the process of condensation and loss by evaporation.

$$dWp/dt = Mcond - Mevpp \quad (37)$$

2.2.1. Moisture flow

The moisture flow at the air of the different components is calculated according to Equation 38 (Monteith, 1972):

$$Mi.j = Dd * Si.j * (Wi - Wj) \quad (38)$$

Where Dd is the coefficient of diffusivity of the water vapour in the air at temperature Tj (C), and can be estimated empirically according to Monteith (1972), using Equation 39:

$$Dd = 2.12E\text{-}03 * (1 + 7E\text{-}03 * Tj) \quad (39)$$

The water flow for cacao beans of the different layers is calculated by Equation 40, where Dp represents the coefficient of diffusivity of water in cacao:

$$Mi.j = Dp * Si.j * (Wi - Wj) \quad (40)$$

The humidity flows that occur from cacao beans to the air by the process of vaporization are calculated by Equation 41. This equation is similar to the one presented by Takakura, Jordan and Boyd (1971) to represent the evaporation of the soil moisture. However, the last term is added to the right, which reduces the evaporation rate as the humidity of cacao beans (Wc) approximates its humidity of equilibrium (Weqc). In this equation Rd represents the resistance to the diffusivity of water in the cacao beans and F1 is a constant, both being determined empirically in the process of the calibration of the model.

$$Mc..a.. = Da/Rd * Sc..a.. * (Wsatc. - Wa.) * (Wc. - Wefc) * F1 \quad (41)$$

The absorption of water of the head space air by the cacao beans of the upper layer is calculated using Equation 42.

$$Mabsct = Da/Rd * Sah.ct * (Wah - Wsatct) \quad (42)$$

Equation 42 is used when the humidty of cacao beans (Wct) is lower than its humidity of equilibrium, calculated in relation to the head space air moisture and when the head space relative humidity is greater than the relation between the vapour pressure in the air of the headspace and the saturation pressure calculated at the cacao temperature. In other situations there will not be an absorption process.

The saturation humidity, the saturation pressure and the vapour pressure used in the equations above, are calculated according to Wilhelm (1976).

The cacao beans equilibrium moisture content is calculated by Equation 43:

$$Weq.c = (k1 * U + k2 * U2 + k3 * U3) * EXP (k4 * U1 + k5 * U2 + k6 * U3 + k7 * U4 * (T+k8)) \quad (43)$$

The flow of condensation of water on the walls of the container, calculated according to Takakura, Jordan and Boyd (1971) is expressed by Equation 44:

$$Mcond = Km * E1 * Sah.p * (Wah - Wsatp) \quad (44)$$

Where E1 is an empirical constant estimated in the calibration of the model.

The water evaporation flow over the walls of the container is calculated by Equation 45.

$$Mevpp = Km * E1 * Sah.p * (Wah - Wsat.p) \quad (45)$$

The water flow due to ventilation is calculated using Equation 46:

$$MVent = Da * Vent * (Wae - Wa) \quad (46)$$

3. The program

The program was written in VSBASIC/IBM used in the CMS interactive environment.

Firstly the program accesses files with information about the characteristics of the container and data on the maximum and minimum external temperatures. The instantaneous temperatures are generated using the functions proposed by Meyer et al. (1976), using values of daily maximum and minimum temperatures.

After calculation of the coefficients of the differential equation the program gives solution to the system using the Euler method. To avoid instability and to reduce the characteristic errors of the integration method used, which occur when the external temperature has sudden variations, the time constant of integration suffers automatic reductions. The time constant typically used in the simulations was 300 seconds.

4. Simulations

Initially the results of the simulations were compared with actual results, obtained by Serôdio and Iturbe (1988). Both researchers travelled on the ship accompanying 4 containers (2 conventional and 2 ventilated) each loaded with 1 500 kg of cacao beans from Ilhéus, Bahia, Brazil to New York, USA. During the trip climatological data at the deck and hold of the ship were registered. Three temperature measurements (9 AM, 3 PM and 9 PM) were taken for each container for the cacao beans of the upper, central, bottom and lateral layers, as well as for relative humidity inside the containers and the humidity of cacao at the upper and bottom layers. Air temperatures from the head space and from the top for each container and the occurrence of the condensation was also registered.

The trip was 14 days but the measurements were continued for 5 more days with the containers delivered at the Port of New York.

As initial values of the model the values of temperature and humidity in each component, registered at the beginning of the trip were used.

The values of the parameters are shown on Table 1.

Table 1 – Values of the parameters used in the simulations.

Simbol	Value	Unity	Reference
Ca	1214.17	$J/m^3.k$	Kreith (1977)
Cp	460.56	J/Kg.k	Kreith (1977)
Da	1.20	Kg/m^3	Kreith (1977)
E	0.85	Kg/m^3	Kreith (1977)
Po	0.54	–	Almeida (1979)
Pp	1000.00	Kg	measured
Pcc	7296.00	Kg	estimated
Pcp	6161.00	Kg	estimated
Pct	1543.00	Kg	estimated
Sah.p	66.08	m^2	measured
Sap.p	39.10	m^2	measured
Sah.p	21.67	m^2	measured
Sah.ct	13.50	m^2	measured
Sep	52.22	m^2	measured
Scc.cp	26.60	m^2	measured
Scc.ct	8.95	m^2	measured
Vc	32.38	m^3	measured
Vah	6.80	m^3	measured
Ji	0.00	–	
Ei	0.02	–	estimated
Fi	1.86	–	estimated
Rd	475.00	s/m^2	Takakura (1971)
Km	4.93E-3	$Kg/m^2.s$	Kreith (1977)
SB	5.67E-8	W/m	Kreith (1977)

Figure 1A represents the simulated and the real temperatures of the ceiling of a traditional container delivered in the ship hold.

Generally, the simulated data is well close to the actual data. On some days mainly on the second, seventh, ninth and nineteenth, the real temperatures at 3 PM were much higher than the simulated values. This difference was acceptable because the model does not take into account the effects of direct sunlight on the container, what could have occurred during the shipment, because of the occasional opening of the hold and when the containers were at port.

Figure 1B represents the real and simulated temperatures of the head space air. The concordance was acceptable. There were differences between the real and simulated values, probably due to the reasons explained in the preceding paragraph.

The graphics in Figure 2 show the real and simulated temperatures of cacao at the upper (2A), peripheric (2B), and central (2C) layer.

The simulated results are a little below to the real results, especially for the period when there is a sudden fall in the external temperature, this divergence

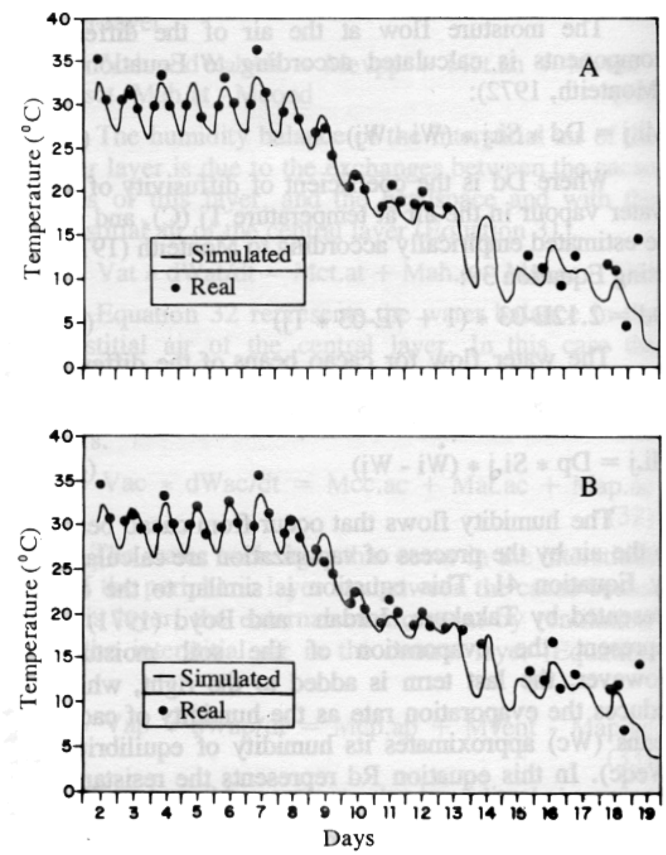

Figure 1 - Simulated and measured real temperatures of the ceiling (A) and of the head space air (B) of a conventional container delivered in the ship's hold.

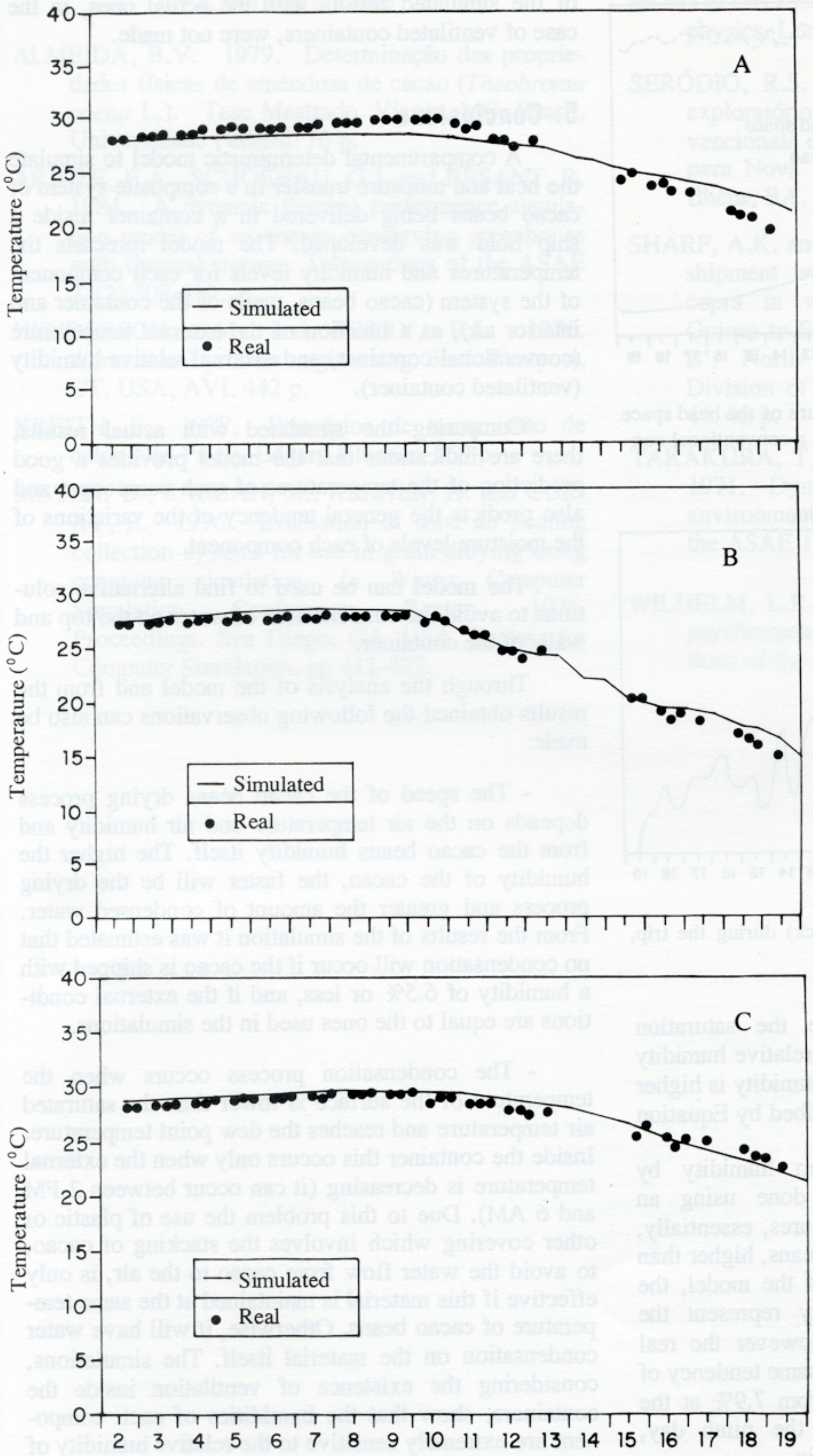

Figure 2. Simulated and measured real temperatures of cacao beans at the upper (A), peripheric (B) and central (C) layer in a conventional container delivered in the ship's hold.

being remarkable for the cacao beans of the upper and peripheric layers. Probably the coefficients of heat transmission between cacao beans and the walls and cacao beans and the head space air are underestimated. It was not possible to find this type of data in the literature.

Statistically, the simulated results in no case differed from the real ones when the chi-square was used.

Figure 3 shows the simulated results of humidity for some components, and the external temperature is represented in Figure 4.

The relative humidity at the headspace air varies with the daily cycle of temperature, at the beginning of the trip. When the external temperature starts down, at the ninth day, the relative humidity maintains high values, then, decreases slowly until the end of the trip. This behaviour was observed in the actual data, although it was not possible to make effective comparisons, since to take the relative humidity measures of the head space air, Serôdio and Iturbe, (1988) opened the doors of the containers and this could have altered the measurements, as recognized by the authors.

At the beginning of the trip with the external temperature heightened, a process of absorption of water by the cacao beans from the upper layer is observed and reaches the maximum value of humidity at the ninth day. From that day the cacao beans start to undergo a slow drying process transfering humidty to the head space air. As the external temperature decreases, the walls of the container cool faster than the internal air, resulting in water condensation on the walls.

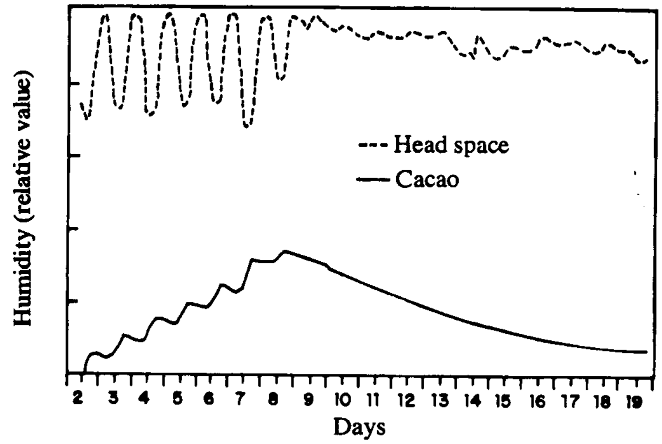

Figure 3 - Simulated results of moisture of the head space air and cacao beans at the upper layer in a conventional container delivered in the ship's hold.

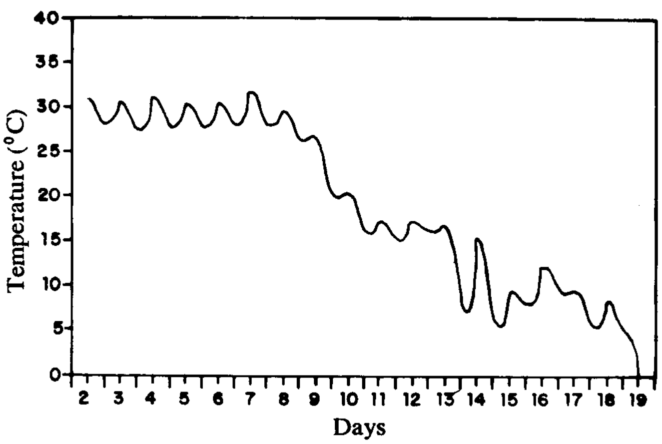

Figure 4 - External temperatures (deck) during the trip, from Ilhéus, Brazil, to New York, USA.

This process continues while the saturation humidity of cacao is higher than the relative humidity of the air and while the cacao beans humidity is higher than its equilibrium humidity as described by Equation 41.

The evaluations of the cacao humidity by Serôdio and Iturbe (1988) were done using an electrical resistance device that measures, essentially, the peripheric humidity of the cacao beans, higher than the internal humidity. In the case of the model, the simulated grades of cacao humidity represent the internal humidity of the product. However the real humidity of cacao beans showed the same tendency of the simulated humidity, increasing from 7.9% at the beginning of the trip to 10% at the ninth day, decreasing to 7.9% at the end of the trip.

Since the sample data taken by Serôdio and Iturbe (1988) did not permit the estimates of instantaneous external relative humidity, comparisons of the simulated results with the actual ones, in the case of ventilated containers, were not made.

5. Conclusions

A compartmental deterministic model to simulate the heat and moisture transfer in a composite system of cacao beans being delivered in a container inside a ship hold was developed. The model forecasts the temperatures and humidity levels for each component of the system (cacao beans, walls of the container and interior air), as a function of the external temperature (conventional container) and external relative humidity (ventilated container).

Comparing the simulated with actual results, there are indications that the model provides a good prediction of the temperatures of each component and also predicts the general tendency of the variations of the moisture levels of each component.

The model can be used to find alternative solutions to avoid the condensation of water on the top and walls of the container.

Through the analysis of the model and from the results obtained the following observations can also be made:

- The speed of the cacao beans drying process depends on the air temperature and air humidity and from the cacao beans humidity itself. The higher the humidity of the cacao, the faster will be the drying process and greater the amount of condensed water. From the results of the simulation it was estimated that no condensation will occur if the cacao is shipped with a humidity of 6.5% or less, and if the external conditions are equal to the ones used in the simulations.

- The condensation process occurs when the temperature of the surface is lower than the saturated air temperature and reaches the dew point temperature. Inside the container this occurs only when the external temperature is decreasing (it can occur between 2 PM and 6 AM). Due to this problem the use of plastic or other covering which involves the stacking of cacao, to avoid the water flow from cacao to the air, is only effective if this material is maintained at the same temperature of cacao beans. Otherwise, it will have water condensation on the material itself. The simulations, considering the existence of ventilation inside the containers, show that the humidities of each component are extremely sensitive to the relative humidity of the external air. When the external humidity is high, the water condensation can occur from the beginning of the trip. With low external humidities, there is no condensation.

Literature cited

ALMEIDA, B.V. 1979. Determinação das propriedades físicas de amêndoas de cacao (*Theobroma cacao* L.). Tese Mestrado. Viçosa, MG, Brasil, Universidade Federal. 70 p.

ARINZE, E.A., SCHOENAU, G.J. and BESANT, R. 1984. A dynamic thermal performance simulation model of an energy conserving greenhouse with thermal storage. Transactions of the ASAE 27(2):508-519.

HENDERSON, S.M. and PERRY, R.L. 1976. Agricultural process engineering. 3 ed. Westport, CT, USA, AVI. 442 p.

KREITH, F. 1977. Princípios de transmissão de calor. São Paulo, Edgard Blucher. 550 p.

MEYER, G., SABBAH, M., KEENER, H. and CURRY, R. 1976. Evaluation of solar air heating collection systems for use in grain draying using computer simulation. *In* Winter Computer Simulation Conference, Boston, 1976. Proceedings. San Diego, CA, USA, Society for Computer Simulation. pp 411-422.

MONTEITH, J.L. 1972. Principles of environmental physics. London, Edward Arnold. 241 p.

SERÔDIO, R.S. e ITURBE, J.R. 1988. Embarque exploratório de cacau usando contentores convencionais e ventilados de Ilhéus (Bahia, Brasil) para Nova Iorque - setembro/outubro de 1987. Ilhéus, BA, Brasil, CEPLAC/CEPEC. 54 p.

SHARP, A.K. and GREVE, J.E. van S. 1984. Trial shipment with bank line of cocoa, coffee and copra in ventilated 'containers', Papua New Guinea to Europe, January/February 1982, 'Trial B'. North Ryde, NSW, Australia. CSIRO. Division of Food Research. Technical Paper nº 44. 42 p.

TAKAKURA, T., JORDAN, K.A. and BOYD, L.L. 1971. Dynamic simulation of plant growth and environment in the greenhouse. Transactions of the ASAE 14(5):964-971.

WILHELM, L.R. 1976. Numerical calculations of psychrometric properties in SI units. Transactions of the ASAE 19(2):318-325.