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Soymilk plant simulation to predict the formula of a new Hypothetical Product

Simulación de una planta de leche de soya para predecir la fórmula de un nuevo producto hipotético

Iacobi Boanerges-Boanerges[1]

ABSTRACT

Ideal Patterns reactors alteration by real reactor patterns, for better accuracy was done using industrial software: Aspen Plus and Hysys Version 7.1 to represent the batch real mixer and soymilk production system. Fluid package for properties prediction was chosen from the software list. A feed steam of 41,67 Kg/h (Soybean) was taken; mass fractions were given by element since the Soybean has a wide blend of substances which cannot be described as a unique compound formula. The elements were **C, N, H, O, S**, **Na, K, Mg, Ca**, **Fe, P, and Cu**. Final flow of 8,333 Kg/h was used to achieve the objective of this study: the elemental analysis method for the hypothetical new product prediction (based only in presence of Amino-acids and other macro and multiple substances). The macromolecules described here are the onset for new specific soymilk compounds such as the concluded on this study. Fulminic Acid Family compound and the protein analysis may correspond to new proteins which are not well-known such as the ones found in studies by the Hospital de Rhode Island in 2014. Presence of Fe and Cu in soybean was ascribed to the micronutrients that could be present in the soil of crop cultivation and in soybeans by absorption.

Keywords: Non-ideal Model Mixer, Soybean, Real Batch Mixer, Hypothetical Molecular formula.

RESUMEN

La alteración de modelos de reactores ideales por modelos reales para mayor precisión fue hecha usando un software industrial: Aspen Hysys Versión 7.1 para representar el mezclador *batch* real y el sistema de producción de leche de soya. El paquete termodinámico de fluidos fue escogido de una de las listas del software. Una corriente de alimentación de 41,67 Kg/h (Soya) fue tomada; las composiciones en fracciones másicas fueron dadas por elemento puesto que las semillas de soya tienen una amplia mezcla de sustancias las cuales no pueden ser descritas como una formula molecular única y sencilla. Los elementos fueron: **C, N, H, O, S**, **Na, K, Mg, Ca**, **Fe, P, y Cu**. El flujo Final de 8,333 Kg/h fue usado para el objetivo de este estudio: El método de análisis elemental para la predicción de un Nuevo posible producto en la composición de la leche de soya (basado solamente en la presencia de amino ácido, y otras macro y múltiples substancias). Las macromoléculas descritas aquí son el inicio para nuevos y específicos componentes de la leche de soya tales como los concluidos en éste estudio. Componente de la familia del ácido fulmínico y el análisis de proteína puede corresponder a nuevas proteínas las cuales no son bien conocidas como la encontrada en los estudios por el hospital de Rhode Island en 2014. La Presencia de Fe y Cu en las semillas de soya fueron atribuidas a los micronutrientes presentes por absorción del suelo del cultivo.

Palabras clave: Modelo no ideal de mezclador, Semilla de soya, Mezclador *batch* real, Formula molecular Hipotética.

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Introduction

Soybean is one of the most economically important crops in the USA whilst in Europe it is very limited, due to climate and soil conditions (A. Geoffrey Norman, 2006). Neither all tank reactors are perfectly mixed, nor do all tanks have their composition and temperature independent from the length of the reactor (Plug-flow behavior – Ideal Reactor) (H. Scott Fogler, 2006). For Soymilk production, this is the case. The latter is an inexpensive source of protein, minerals, carbohydrates, oil (blends), vitamins and calories for human consumption. All its compounds formula have not been described completely due to the different species and varieties in the world and their chemical variation such as the well-known health benefits: Proteins, Isoflavones, and dietary fibre (glucose, uronic acids, galactose, arabinose and xylose) – (Ren, Liu, Endo, Takagi & Hayashi, 2006). Moreover, Soymilk is a low-cost substitute for dairy milk for the poor in the developing countries. Being free of cholesterol, gluten and lactose, soymilk is also a suitable food for lactose-intolerant consumers, vegetarians and milk-allergy patients. Today, consumer demands are more and more directed toward high-quality, additive free, minimally processed, nutritious, and deteriorative

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organisms as well as inactivate undesirable enzymes (Seibel & Beleia, 2009). Nevertheless, high pasteurization temperatures impact negatively on the nutritional quality and taste of milk (Chou & Hou, 2010). Soybean seeds are known to contain different anti-nutritive factors, such as: trypsin inhibitors, phytic acid, raffinose and stachyose many of which lose their effects after processing. Previous research (Becker-Ritt, Mulinari, Vasconcelos, & Carlini, 2004; Kumar, Rani, Solanki, & Hussain, 2006) shows that there is an increasing interest from scientists in soybean which is focused on the characterization of its components. The aim of this paper is attain new data and information about the Soymilk composition which may be relevant to the scientific and industrial – health community, using a Simulation Aspen Hysys software which has customer testimonials from: **LG Chemistry, Chevron, Arithmetek, Siam, Petro-bras, Campbell, ConocoPhillips, Fluor, Hitachi Zosen, Genesis Consulting, INEOS and others (Fusco, 2013).** The macromolecules described here are the onset for new specific soymilk compounds.

Materials and methods

Soybean samples and water extract of soybeans (soymilk)

0,5 Kg/h were feedstock for the process resembling the one undergone in markets in Brazil and Canada, taking care to ensure that good quality of soybeans (Chemical composition). Whole soybeans were first washed and soaked with hot water and undergo pre-heating, to inactivate the Lipoxigenase to foresee bad properties in the final flavor, until the water boiling point (at 89,326 KPa) – (CDMB 2013) for 5 min. The soybeans were blended with 2 times of volume of soybean in water, then the soybeans were taken in a **grinding unit** for 3 minutes. Then the mixture of soybean was filtered in a 1,2 µm filter. The solid residue was used to measure the PH between 8 and 8,5 in two measures. The final liquid filtered was heated (138 °C) before entry to the pasteurization process 600 MPA and (148 °C) streamed to a container at -2 °C and 89.326 KPa in 3 seconds (**Figure 1**).

Soybean composition and Soybean composition prediction.

Table 1. Chemical composition prediction through the software for soybeans

Compound	Mass Fractions	Vapour Phase	Aqueous Phase	Solid Phase
Proline	0,000000	0,000000	0,000000	0,000000
Valine	0,000000	0,000000	0,000000	0,000000
Niacin	0,000000	0,000000	0,000000	0,000000
Thiamin	0,007406	0,000000	0,137357	0,000000
Stachyose	0,000000	0,000000	0,000000	0,000000
Raffinose	0,000000	0,000000	0,000000	0,00000
Sucrose	0,000000	0,000000	0,000000	0,00000
Daldzein	0,000000	0,000000	0,000000	0,00000
Cu - Copper	0,000001	0,000000	0,000057	0,00000
Calcium	0,002129	0,000000	0,000000	0,004125
Carbon	0,479430	0,000000	0,000000	0,928818
Nitrogen	0,136082	0,291030	0,000209	0,000000
Oxygen	0,263397	0,563316	0,000294	0,000000
Sodium	0,000009	0,000020	0,000005	0,000000
Magnesium	0,002037	0,000000	0,125306	0,000000
Phosphorus	0,005369	0,002800	0,249787	0,000000
Iron Fe	0,000087	0,000186	0,000000	0,000000
Potassium	0,017589	0,037344	0,007849	0,000000
Water	0,019070	0,024131	0,479102	0,000000
Hydrogen	0,032781	0,070108	0,000034	0,000000
Sulfur				
S_Rhombic	0,034613	0,000000	0,000000	0,067057
Total	1,000000			

Source: Software Aspen Tech Hysys v 7.1

In this Stage of the process, 3 units were included (Heating, Pasteurization and Cooling) to guarantee the quality of the food by the microorganism inactivation. The fluid packages fo this stage were the Generic COMthermo Pkg. (Van Laar – Virial for Liquid blends) and extended NRTL- Virial (For Soybean Solid properties and Pasteurization Final Product). The heating unit was included to prevent damage due to the high increase of the temperature at Pressure values of 600 MPa. Since an increase (DT = 123 °C and DP = 498675 Pa) is furnish for the entire process, the latter was caused by the collisions of the particles. Besides, the Heat supply from the heat source makes necessary a rigorous and strict control for the temperature, the Heating unit at 101,325 KPa is a cheaper alternative. In this stage, the condition for the inlet and outlet streams can be appreciated including the duty (Heat Flux) 3,766 KJ/h. The unit of cooling is included to guarantee the inactivation of pathogenic microorganism by the collision of hot particles (148 °C) with a container with fluid at -2 °C value.

Table 2. Thermodynamics properties for the soybeans after Pre-Heating Stage (Inactive Lipoxygenase)

Stream Name	Soybean Enzymes	Vapour Phase	Liquid Phase	Solid Phase
Vapour /Phase Fraction	0,4004	0,4004	0,0020	0,5976
Temperature (Kelvin)	373,15	373,15	373,15	373,15
Pressure (Kpa)	101,30	101,30	101,30	101,30
MolarFlow (kgmole/h)	2,6830 E-02	1,0560 E-02	5,3030 E-05	1,5770E-02

MassFlow (kg/h)	0,5000	0,3085	0,0014	0,1901
Std Ideal liqvol Flow (m^3/h)	4,6060 E-04	3,4370 E-04	1,0090 E-06	1,1590E-04
MolarEnthalpy (KJ/ Kgmole)	-4771	-12670	-162900	1054
MolarEntropy (KJ/ KgmoleC)	65,79	154,8	-382,7	7,685
HeatFlow (KJ/h)	-125,9	-133,8	-8,637	16,61
LiqVol Flow@ StdCond (m^3/h)			9,6510 E- 07	1,1590E- 04

Source: Software Aspen Tech Hysys v 7.1

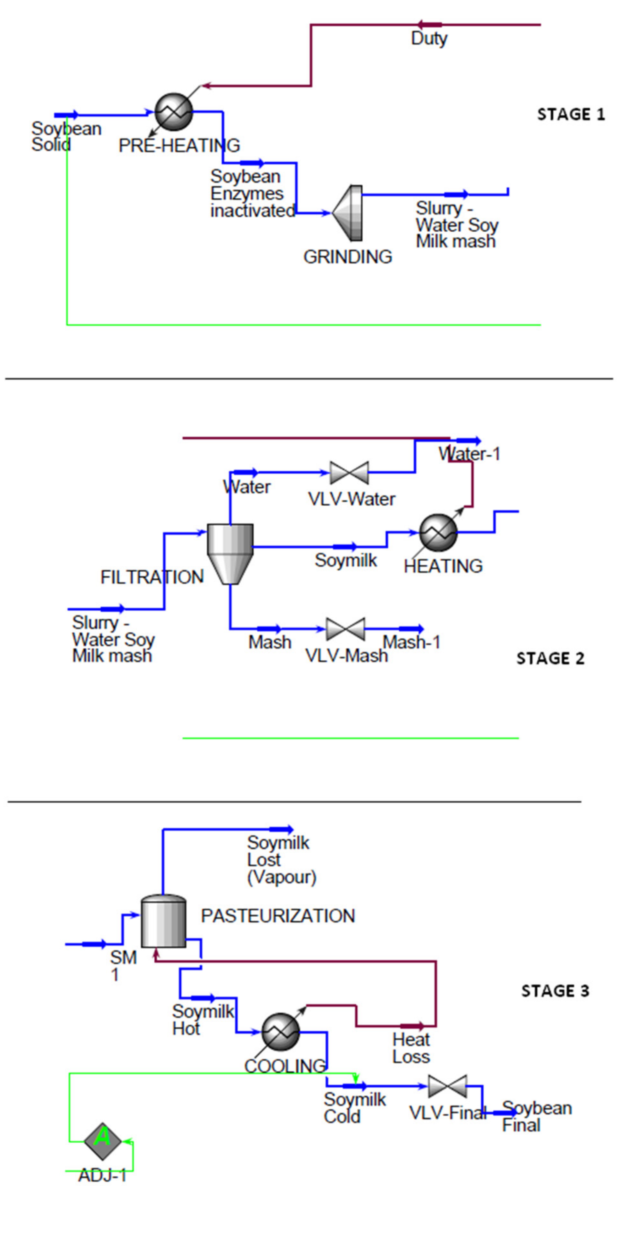

Figure 1. - Soymilk Production, Plant Simulation by Aspen Hysys
Source: Aspen Tech Hysys v 7.1 – Flow sheet panel

Stage1, 2 and 3 are continuously linked in a unique flow sheet diagram (Figure adapted for the journal template)

Results and discussion

Element composition and soymilk compounds

The final soymilk was formed by 16 amino-acids, the Polysaccharides stachyose, Rafinosse, Sucrose, Daidzein as the total isoflavones, and thiamin and niacin as Vitamin B content. The final mass fractions of Carbon **wC = 0.002455**, Nitrogen **wN = 0.005726**, and **Oxygen wO = 0.006541**, **Copper wCu = 0,012988**, **Calcium wCa = 0,008193**, **Sodium wNa = 0,004699**, **Magnesium wMg = 0,004968**, **Phosphorus wP = 0,006632**, **iron wFe = 0,011416**, **Potassium wK = 0,007992**, **Hydrogen wH = 0,000412**, **Sulfur wS = 0,006555** indicate a presence of macromolecules besides the cited above, which chemical Structures can be derived from the empirical formula and subsequently by the Global molecular formula.

Table 3. Pasteurization Thermodynamics conditions for UHT and UHPH units

Name	SM 1	Soymilk Hot	Soymilk Lost (Vapour)	HeatLoss
Vpour/PhaseFraction	0,1359	0,1111	0,2956	
Temperature (Celcius)	138	148	100	
Pressure (Kpa)	101,3	101,3	6,00E+05	
Molar Flow (kgmole/h)	2,78 E-02	6,61E-04	3600	
Mass Flow (kg/h)	4,088	0,1000	2,94E+05	
Std Ideal liqvol Flow (m^3/h)	3,01 E-03	7,35E-05	225,9	
Molar Enthalpy (KJ/Kgmole)	-3,17 E+05	-3,66 E+05	-1,73E+05	
MolarEntropy(KJ/Kgmole*C)	-6455	-6903	-4101	
Heat Flow (KJ/h)		-241,8	-6,24E+08	-3,756

Source: AspenTech Hysys – Flowsheet Conditions

Global molecular formula assessment

(For t = 1 hour) Source data: Table 4

mi = mt * wi
Equation (**1**) **– Mass calculation for each component**

mi = mass of each element
mt= total mass
wi = mass fractio

Equation (**2**) **– Mole calculation for each component**
For Carbon replacing (1) e.g.

mc = mt * wc

Equations and calculation procedure

$$mC = 8{,}3333\ \frac{kg}{h} * (0{,}002455) = 0{,}020458\ \frac{kg}{h} \qquad (1.1)$$

$$mole\ C = \frac{0{,}020458\ kg}{12{,}0115\ kg/mole} = 0{,}001703\ kmole \quad (2.1)$$

$$mN = 8{,}3333\ \frac{kg}{h} * (0{,}005726) = 0{,}047716\ \frac{kg}{h} \quad (1.2)$$

$$mole\ N = \frac{0{,}047716\ kg}{14{,}0071\ kg/mole} = 0{,}003407\ kmole \quad (2.2)$$

$$mCa = 8{,}3333\ \frac{kg}{h} * (0{,}008193) = 0{,}068275\ \frac{kg}{h} \quad Eq(1.3)$$

$$mole\ Ca = \frac{0{,}068275\ kg}{40{,}0784\ kg/mole} = 0{,}001704\ kmole \quad (2.3)$$

$$mK = 8{,}3333\ \frac{kg}{h} * (0{,}007992) = 0{,}066600\ \frac{kg}{h} \quad (1.4)$$

$$mole\ K = \frac{0{,}068275\ kg}{40{,}0784\ kg/mole} = 0{,}001703\ kmole \quad (2.4)$$

$$mMg = 8{,}3333\ \frac{kg}{h} * (0{,}004968) = 0{,}041400\ \frac{kg}{h} \quad (1.5)$$

$$mole\ Mg = \frac{0{,}041400\ kg}{24{,}3051\ kg/mole} = 0{,}001703\ kmole \quad (2.5)$$

$$mCu = 8{,}3333\ \frac{kg}{h} * (0{,}012988) = 0{,}10283\ \frac{kg}{h} \quad (1.6)$$

$$mole\ Cu = \frac{0{,}041400\ kg}{24{,}3051\ kg/mole} = 0{,}001703\ kmole \quad (2.6)$$

$$mO = 8{,}3333\ \frac{kg}{h} * (0{,}006541) = 0{,}054508\ \frac{kg}{h} \quad (1.7)$$

$$mole\ O = \frac{0{,}054508\ kg}{15{,}9994\ kg/mole} = 0{,}003407\ kmole \quad (2.7)$$

$$mFe = 8{,}3333\ \frac{kg}{h} * (0{,}011416) = 0{,}095133\ \frac{kg}{h} \quad (1.8)$$

$$mole\ Fe = \frac{0{,}095133\ kg}{55{,}8452\ kg/mole} = 0{,}001704\ kmole \quad (2.8)$$

$$mP = 8{,}3333\ \frac{kg}{h} * (0{,}0006632) = 0{,}055266\ \frac{kg}{h} \quad (1.9)$$

$$mole\ P = \frac{0{,}055266\ kg}{30{,}97376\ kg/mole} = 0{,}001784\ kmole \quad (2.9)$$

$$mNa = 8{,}3333\ \frac{kg}{h} * (0{,}004699) = 0{,}055266\ \frac{kg}{h} \quad (1.10)$$

$$mole\ Na = \frac{0{,}055266\ kg}{30{,}97376\ kg/mole} = 0{,}001703\ kmole \quad Eq\ 2.10$$

$$mH = 8{,}3333\ \frac{kg}{h} * (0{,}000412) = 0{,}003433\ \frac{kg}{h} \quad Eq\ 1.11$$

$$mole\ H = \frac{0{,}003433\ kg}{1{,}00797\ kg/mole} = 0{,}003406\ kmole \quad Eq2.11$$

$$mS = 8{,}3333\ \frac{kg}{h} * (0{,}006555) = 0{,}054625\ \frac{kg}{h} \quad Eq\ 1.12$$

$$mole\ S = \frac{0{,}003433\ kg}{1{,}00797\ kg/mole} = 0{,}001704\ kmole \quad Eq\ 2.12$$

After dividing all moles in 0,001703 k-mole to find the mole empirical ratio we obtain:

$C\ H_2S\ N_2O_2$

$Cu\ Ca\ Na\ Mg\ P_{1,05}\ Fe\ K$

We must find a ratio of integers according to the law of mass action.

Table 4. Final Element composition of soymilk (compounds sheet)

Compound	Mass Fractions	Vapour Phase	Liquid Phase	Solid Phase
Aspartic Acid	0,027208	0,000321	0,029642	0,000000
Glutamic Acid	0,030076	0,000093	0,032784	0,000000
Serine	0,021483	0,000007	0,023421	0,000000
Histidine	0,031716	0,000073	0,034574	0,000000
Threonine	0,024350	0,000062	0,026544	0,000000
Arginine	0,035609	0,001527	0,038715	0,000000
Alanine	0,018212	0,000025	0,019854	0,000000
Tyrosine	0,037038	0,000044	0,040378	0,000000
Cystine	0,049121	0,030068	0,051405	0,000000
Methionine	0,030501	0,000252	0,033236	0,000000
Phenylanine	0,033768	0,000351	0,036791	0,000000
Isoleucine	0,026814	0,000011	0,029234	0,000000
Leucine	0,026814	0,001408	0,029134	0,000000
Lysine	0,029883	0,000178	0,032568	0,000000
Proline	0,023535	0,000303	0,025637	0,000000
Valine	0,023947	0,000458	0,026076	0,000000
Niacin	0,025166	0,000094	0,027431	0,000000
Thiamin	0,061490	0,213281	0,051788	0,000000
Stachyose	0,136259	0,010555	0,147805	0,000000

Raffinose	0,103112	0,001424	0,112318	0,000000
Sucrose	0,069971	0,085997	0,070137	0,000000
Daldzein	0,051969	0,017003	0,005544	0,000000
Cu - Copper	0,012988	0,182700	0,001094	0,000000
Calcium	0,008193	0,000000	0,000000	0,476240
Carbon	0,002455	0,000000	0,000000	0,142723
Nitrogen	0,005726	0,087266	0,000002	0,000000
Oxygen	0,006541	0,099635	0,000006	0,000000
Sodium	0,004699	0,022191	0,003537	0,000000
Magnesium	0,004968	0,000000	0,005417	0,000000
Phosphorus	0,006322	0,002827	0,006701	0,000000
Iron Fe	0,011416	0,171955	0,000148	0,000000
Potassium	0,007992	0,040176	0,005840	0,000000
Water	0,003683	0,023443	0,002338	0,000000

Source: Aspen tech Hysys v. 7.1

$$C_{20}\ H_{40}\ S_{20}\ N_{40}\ O_{40}\ \textit{(Macro-molecule)}$$

$$Cu_{20}\ Ca_{20}\ Na_{20}\ Mg_{20}\ P_{21}\ Fe_{20}\ K_{20}\ \textit{(Mineral ratio)}$$

Table 4. Final Element composition of soymilk (compounds sheet)

Hydrogen	0,000412	0,006274	0,000001	0,000000
Sulfur S_Rhombic	0,006555	0,000000	0,000000	0,381037
Total	1,000000			

Source: Aspen tech Hysys v. 7.1

Conclusions

Based in the composition predicted by the software, we can make a classification of the specie for the soybean (Glycine Max. L.). It resulted in the presence of $\mathbf{C_{20}\ H_{40}\ S_{20}\ N_{40}\ O_{40}}$ that indicates the presence of Protein (the presence of an essential amino acid with sulfur). Multiple **Biomolecule** options can be derived from this analysis such as: Organometallic Compounds, OrganoPhosphorus Compounds, Proteins, Carbohydrates, Fat, Vitamins. One option for this could be large linear chains with methionine or cysteine both considered as unique source. **1,1111 mole of $C_8H_{18}N_2O_4S_2$ or a 1 mole of $(CH_2(NO)_2)_{20}$ (Fulminic Acid Family compound)** according to (H Yang & L. Zhang, 2007), and an Organ phosphorus compound (Phospholipids). Although this last one is present mostly in pesticides, two hypothesis can be considered: The presence of them due to residuals in soybean after chemical process in a non-mortal level, or their presence as any of these compounds: **$P(=O)(OR)_3$; $RP(=O)(OR')_2$; $R_3P=O$;.** According to (Seibel & Beleia 2009), one kind is $\mathbf{C_6H_{18}O_{24}P_6}$ written as $\mathbf{(C_2H_6)_3(O_4P)_6}$ (phytic acid) where the remaining 15 atoms of P would be inorganic Phosphorus. The remaining proportions of mole for protein analysis may correspond to new proteins which are not well-known such as those found in studies by the Hospital de Rhode Island (Jonathan Kurtis, 2014 PfSEA-1 2014 Journal: Science) for the presence of trace elements (Micronutrients – trace elements Cu and Fe) (Organometallic compounds).

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