MODELLING MEALINESS DYNAMICS IN APPLES WITH EcosimPro AS RELATED TO TEXTURE PARAMETERS

Barreiro P[1]; Verlinden B. E[2]; De Smedt V[2]; Nicolai B[2]; Ruiz-Altisent, M[1]

Physical Propeties Lº; Rural Engineering Dept; ETSIA-UPM, Madrid, Spain
Flanders Centre/Laboratory of Postharvest Technology. Catholic University Leuven, Belgium

Abstract: Mealiness is a texture disorder associated to a lack of crispiness, hardness and juiciness. Such texture parameters may be assessed through related mechanical properties (shear resistance, elasticity modulus...), and modelled through a complex system combining biochemical reactions and water transport phenomena. Well defined metabolic reactions such as respiration, starch hydrolysisand middle lamella solubilisation are combined with turgor loss and tissue dehydration to extract consequences on the development of mealiness.
The mechanistic model which already has been identified on Cox's Orange Pippin data has been fitted in this paper to data from apples cv. Golden and Top-Red corresponding to different harvest dates and storage conditions A sensitivity analysis has been carried out.

Keywords: EcosimPro, fruit quality, dynamic behaviour, simulation, kinetic control system

1. INTRODUCTION

Overall acceptance of fruits by consumer relies on taste and flavour aspects, as well as on texture properties. The first ones depend upon the chemical composition, while the latters are assumed to be dependent on the amount and characteristics of structural polysaccharides.

Attempts have been carried out to model the dynamic behaviour of several chemical compounds such as sugars. Hertog et al. in 1997 modelled sugar evolution in potato tubers as a compromise between starch degradation and respiration. Tijkens et al. in 1997 developed a dynamic model that describes the decrease of firmness in apples as affected by chemical and biochemical reactions. Also, dynamics of enzymatic reactions concerning structural polysaccharides as affected by heat treatments have been modelled by Verlinden and De Baerdemaeker (1997) on carrot tissue. These authors also established a link between macroscopic mechanical behaviour observed in carrot tissue submitted to tensile stress and the amount of middle lamella and percentage of broken cell in the tissue.

Besides the above mentioned research studies, little work has been done to clarify how biochemical reactions related to non structural components, as well as water movement may indirectly affect mechanical properties and, therefore, texture perception.

Mealiness is a textural attribute defined by Jowitt in 1974 as: "possessing the textural property manifested by the presence of readily separated laminar structural elements". At a microscopic level, De Smedt et al. in 1998 confirmed that the broken surface of mealy tissue shows a lower amount of broken cell as well as more rounded shape of cells. That study has been carried out under the scope of a European Project (FAIR-CT95-0302: 'Mealiness in fruits. Consumer perception and means for detection') where this textural disorder has been faced under a broad range of points of view. One of those aspects has been the development of instrumental procedures for mealiness assessment with regard to sensory definition (Barreiro et al., 1998 a & b). In these studies, mealiness has revealed to be a multidimensional sensory parameter related to the lack of crispness, of hardness and of juiciness. Those unidimensional sensory parameters may be assessed through shear rupture and confined compression tests on fruit probes.

Another field of work within referred European Project, has to do with identifying field and storage conditions that enhance mealiness onset (Barreiro 1998a, De Smedt 2000). In general, late picking dates and large fruit sizes, non controlled atmosphere and high relative humidity positively affect the development of mealiness..

Finally, one of the major results of above mentioned European Project has been the formulation of a mechanistic model concerning biochemical reactions on structural and non structural polysaccharides and water transport. The state variables of this model are linked to instrumental crispness, hardness and juiciness. This model which will be outlined in this paper

has been shown to fit successfully data of Cox's Orange Pippin apples subjected to different storage conditions (De Smedt, 2000).

2. OBJECTIVES

The objective of this research was to apply a dynamic model concerning sugar metabolism, water transport and middle lamella solubilisation to simulate and to get a better understanding of the consequences of factors affecting mealiness development in *Top-Red* and *Golden* apples.

3. MATERIAL AND METHODS

Apples cv *Golden and Top-Red* were studied for mealiness assessment. Apples were grown in Lérida, the main area of pome fruit production in Spain by UdL-IRTA according to the following full factorial experimental design: ***1) Harvest dates***: three different dates of harvest corresponding to early, common and late harvest dates from 1996 season, ***2) size of the fruit***: two different sizes: diameter < 75mm and > 75mm, ***3) storage temperature:*** three different temperatures have been tested under non-controlled atmosphere: -0.5, +0.5 and 2 ºC, and ***4) storage period:*** three different modalities have been tested for this factor: at harvest, 3 month storage and 6 month storage. Apples were stored in commercial chambers. A total amount of 420 fruits were tested per cultivar. The tests carried out on these samples can be summarised as follows:

- Mechanical tests:

- Confined compression test: carried out with a universal testing machine on cylindrical probes of 1.7 cm height and 1.7 cm diameter. Probes were confined in a disc of 1.7 cm height, with a hole of the same diameter as the probe. A maximum deformation of 2.5 mm was applied at 20 mm/min speed rate. The rod used in this test had a 15.3 mm diameter in order to avoid rod/disc contacts during compression. Deformation was immediately removed at the same speed rate; one repetition was made per fruit. The following parameters were registered through these tests: 1) Force/deformation ratio within the elastic range (N/mm, CFD) which is proportional to Young´s Modulus and which will be used as instrumental hardness; and 2) Juice area (mm^2, JUICE) of the spot accumulated in a filter paper placed underneath the probe during the test, which will be used as compression juiciness (Paoletti et al. 1993)
- Shear rupture test: To perform this test a special device developed in 1992 by Jarén and Ruiz-Altisent was used. This test was carried out on probes of 1.4 cm diameter and 2.0 cm height. An increasing deformation was applied at a 20mm/min speed rate until probe rupture was achieved; one repetition was carried out per fruit. The maximum force (strenght, SF) at the shear rupture point was registered, which will be used as shear crispness (N) (Paoletti et al. 1993)

- Chemical measurements: soluble solids content (SSC) was measured by a digital refractometer PR-101 ATAGO, and titratable or total acidity (meq/l) by titration using NaOH 0.1 N and a phenolphtalein indicator.

4. MODEL STRUCTURE

The development of model structure has been reported by De Smedt (2000, see Figure 1). An apple is a very complex system which can be summarised as a pool of six state variables subject to biochemical reactions (respiration, starch hydrolysis and middle lamella solubilisation), and water transport phenomena. The apple is assumed to consist of two compartments (the cell and the intercellular space) which are separated by a semi-permeable membrane. Intercellular space may also exchange water with the environment via epidermal transport. State variables and dynamic behaviour are summarised in Table 1.

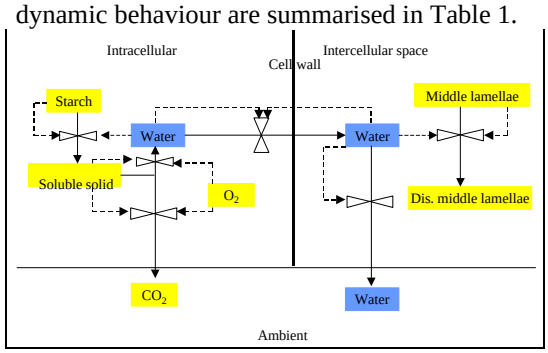

Figure 1. Schematic representation of the model

The output relations - the relationships between state variables and macroscopic behaviour such as instrumental crispness, hardness, juiciness and soluble solids - are summarised in Table 2.

The model contains 14 parameters to be estimated. However, many have been bounded by means of literature data (See Table 3); see Table 4 for model notation.

5. SIMULATION WITH ECOSIMPRO

Numerical integration was carried out with ECOSIMPRO. The model contains six state variables and two boundary conditions which are all included in a single component.

CONST REAL Rgas = 8.314
CONST REAL MW_S = 180.

```
CONST REAL MW_H = 180.
CONST REAL MW_P = 194.
CONST REAL MW_L = 194.
CONST REAL MW_H2O = 18.

FUNCTION NO_TYPE DISCR(OUT REAL x)
  BODY
    RETURN
END FUNCTION

COMPONENT applecordef
  DATA
    REAL ks = 4.63e-07
    REAL kh = 1.39e-08
    REAL kl = 1.22e-07
    REAL hmc_Ac = 3.47e-12
    REAL hmi_Ai = 6.94e-14
    REAL Eo = 1.00e5
    REAL a = 9.33e6
    REAL b = 3.00e+01
    REAL c = 1.61e+01
    REAL d = 2.63e+00
    REAL e = 3e-06
    REAL f = 6.77e-01
    REAL g = 8.8e+07
    REAL Ap = 2.27e-4
    REAL lp = 17
    REAL Nc=6.6e7


  DECLS
    BOUND REAL T
    BOUND REAL phi
    REAL B
    REAL E
    REAL H
    REAL L
    REAL P
    REAL PSI_c
        REAL PSI_pc
        REAL PSI_pic
    REAL PSI_i
    REAL PSI_amb
    REAL S
    REAL Wc
    REAL Wi
    REAL m_apple
    REAL m_apple_o
    REAL weight_loss
    REAL SF
    REAL CFD
    REAL Vw
        REAL VH
        REAL VS
        REAL V
    REAL JUICE
    REAL Lo
    REAL Po
        REAL SSC – añadido
    REAL days

  INIT
    m_apple_o =  S * MW_S + H * MW_H + L *
MW_L + P * MW_P + \
          Wc * MW_H2O + Wi * MW_H2O
    Lo = L
    Po = P
  CONTINUOUS
    DISCR(m_apple_o)
    DISCR(Lo)
    DISCR(Po)
    --Hydrolisis of starch
    S' = - ks * S * Wc / ( S + H + Wc)
    --Oxidation of sugars
    H' = - kh * H + ks * S * Wc / ( S + H + Wc)
    --Hydrolisis of the middle lamella
    L' = - kl * L * Wi / (L + P + Wi)
    P' =  kl * L * Wi / (Lo + Po + Wi)
    --Water balance in the cell
    Wc' =  6 * kh * H - ks * S * Wc / (S + H + Wc)\
- hmc_Ac * (PSI_c - PSI_i)
    --Water balance in the  intercellular space
    Wi' = hmc_Ac *(PSI_c - PSI_i) - hmi_Ai \
* (PSI_i – PSI_amb) - kl * L * Wi / (Lo + Po + Wi)
    Vw = MW_H2O / 1e6
    VH = MW_H / 1e6
    VS = MW_S / 1e6
    V = (H * VH + Wc * Vw + S * VS)/Nc
    PSI_c = PSI_pic + PSI_pc
    PSI_pc = a - b * V**(-1/2)
    PSI_pic = Rgas * T / Vw  * log(Wc / (Wc + H \
+ S))
    PSI_i = Rgas * T / Vw * log(Wi / (Wi + P + L))
    PSI_amb = Rgas * T / Vw * log(phi/100)
    --Output variables
    B = L / (Lo + Po)
    JUICE = c * (Wi + B * Wc)
    SF = d * exp(e * PSI_pc)
    E = Eo + f * PSI_c + g * L
    CFD = (Ap / lp)  * E
    SSC = H * MW_H * 100 / (Wc * MW_H2O
    weight_loss = 100 * (m_apple_o - m_apple) /
m_apple_o

    m_apple = S * MW_S + H * MW_H + L *
MW_L + P * MW_P + \
          Wc * MW_H2O + Wi * MW_H2O
    days = TIME / 3600. / 24.
END COMPONENT
```

6. PARAMETER ESTIMATION

Manual fitting of initial values and model parameters was carried out for two extreme harvest dates of big size *Golden* apples (see Figure 2 and Table 5). These sets of data have been selected from a pool of 9 available for big size *Golden* apples (3 harvest dates × 3 storage temperatures). All predicted values match the experimental to a tolerance level below the

standard error of the experimental data, however the low amount of experimental data points does not allow a proper estimation of all parameters. Therefore, at this stage the model should only be considered as qualitative.

A comparison between fitted values for early and late harvested, big size, Golden apples (see Table 5) indicated that late harvested apples have less starch (S_0) and higher hexose (H_0) content, as well as a higher respiration rate (k_H) than early picked apples. For this set of data, the amount of non solubilised middle lamella was lower for late harvested apples ($L_0$3) though it was also degraded at a slower rate (k_L) than early picked apples.

In the current mechanistic model it is assumed that:

- The instrumental crispiness (*SF*) only depends on the turgor potential of the cell (Ψ_p),
- The instrumental hardness (*CFD*) is mainly related to the amount of non solubilised middle lamella (*L*) and to a less extent to the turgor potential (Ψ_p) and other tissue structures (approximately 65%, 30% and 5% of total hardness, respectively),
- juiciness (*JUICE*) relies to approx. 90%. on the combination of water inside the cells (W_c) and the percentage of broken cells (*B*) during loading. Water in the intercellular spaces completes the contribution to juiciness, and
- the soluble solids content is proportional to the ratio hexose (*H*) to water inside the cells (W_c), therefore the combination of turgor loss and respiration is critical for the dynamics of soluble solids.

Simulation of the dynamics of the state variables and the desired outputs (instrumental crispiness, hardness, juiciness and soluble solids) were carried out in early harvested Golden apples for different relative humidity levels of the ambient (95 & 99% RH) and respiration rates of the cell ($0.1\times k_H$ to k_H, see Figure 3). As expected, relative humidity had a large effect on the transpiration rate: water is pumped from the cell to the intercellular spaces, and the turgor and instrumental crispiness decrease correspondingly. The slight effect of the RH on instrumental hardness was also due to turgor loss.

An interesting feature derived from current mechanistic model was the effect of some chemical compounds such as the amount of hexose units on the evolution of some textural parameters as instrumental crispiness and hardness. A high respiration rate showed to promote the loss of osmotic potential inside the cell allowing a decrease in turgor, and therefore a decrease in instrumental crispiness. As a consequence, there was an increase of water in the intercellular spaces which allowed a slightly higher degradation rate of the middle lamella than for lower respiration rates, and therefore instrumental hardness also decreased. The range of respiration rate which was used ($0.1\times k_H$ to k_H) appeared to be low when compared to the maximum range found for a mechanistic model of respiration on potatoes ($0.1\times k_H$ to $10\times k_H$), Hertog et al., 1997) so even greater effects could be expected in reality.

The effect of the respiration rate on the soluble solids content was comparable to that of the relative humidity of the ambient. A high relative humidity (low water loss) combined with a high respiration rate may lead to a significant decrease in soluble solids which was not found for low relative humidity conditions under the same respiration rate.

Most kinetic parameters of Top Red apples matched with those of Golden.

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Table1. Model summary. See Table 4 for notation.

$$\frac{\mathrm{d}S}{\mathrm{d}t} = -k_s S \frac{W_c}{S + H + W_c}, \text{ with } S_n(t=0) = S_{n0}$$

$$\frac{\mathrm{d}H}{\mathrm{d}t} = +k_s S \frac{W_c}{S + H + W_c} - k_h H, \text{ with } S(t=0) = S_0$$

$$\frac{\mathrm{d}L}{\mathrm{d}t} = -k_l L \frac{W_i}{L_0 + P_0 + W_i}, \text{ with } L(t=0) = L_0$$

$$\frac{\mathrm{d}W_c}{\mathrm{d}t} = +6k_h H - k_s S \frac{W_c}{S + H + W_c} - h_{mc} A_c \left(\Psi_c - \Psi_i\right) \text{ with } W_c(t=0) = W_{c0}$$

$$\frac{\mathrm{d}W_i}{\mathrm{d}t} = h_{mc} A_c \left(\Psi_c - \Psi_i\right) - h_{mi} A_i \left(\Psi_i - \Psi_\infty\right) - k_l L \frac{W_i}{L_0 + P_0 + W_i}, \; W_i(t=0) = W_{i0}$$

Table 2. Intermediate and desired outputs of the model.

$B = L / (L_o + P_o)$	$JUICE = c * (W_i + B * W_c)$	$SSC = (H * M_H * 100) / (W_c * M_W)$
$SF = d \exp (e \psi_{pc})$	$CFD = A_p/l_p * (E_o + f * \psi_{pc} + g*L)$	

Table 3. Data extracted from bibliography to bound the range of variation of state variables, intermediate outputs and model parameters

$W_c + W_i$	85% of fresh weight or 47 moles per kg fresh weight (Belitz & Grosch, 1997)
H + S	11% of fresh weight or 0.6 moles per kg fresh weight (Belitz & Grosch, 1997)
P + L	0.6% of fresh weight or 0.03 moles per kg fresh weight (Belitz & Grosch, 1997)
A_c	6.45 m2 per kg fresh weight (derived from Reeve, 1953)
k_S	0.0161 – 0.0033 1/day

	k_H	8.39 10-5 – 1.53 10-2 1/day(Hertog et al., 1997)
	ψ_p	0.54 to 1.13 Mpa (Harker & Hallet, 1992) it becomes 0 for an approximate relative water content of 80% (Hall et al., 1993)
	ψ_π	-1.33 to –1.8 Mpa (Harker & Hallet, 1992)
	B	80 to 40% for fresh and mealy tissue respectively (De Smedt et al., 1998)

Table 4. Notation

A_c , A_i	(m^2/kg f.w.)	Specific cell membrane area and Specific apple surface area
A_p	(m^2)	Cross section of the probe used for the confined compression test
b	(N/sqrt m)	Coefficient
B	(-)	Broken cell index
c	(mm² kg f.w./mole)	Coefficient
d	(-)	Coefficient
e	(m^2)	Coefficient
E_0	(N/m²)	Reference Elasticity modulus of the apple flesh
f	(-)	Coefficient
g	(N kg.fr.wt/m^2 mole)	Coefficient
H	(mole/kg f.w.)	Moles of hexose per kg f.w. apple tissue
$h_{m,c}$	(mole/m^2.Pa.s)	Mass transfer coefficient of water transport through the cell wall
$h_{m,i}$	(mole/m^2.Pa.s)	Mass transfer coefficient of water transport through the intercellular space to the ambient
k_L	(1/s)	Rate constant for middle lamella degradation
k_H	(1/s)	Rate constant for sugar oxidation
k_S	(1/s)	Rate constant for starch hydrolisation
L	(mole/kg f.w.)	Moles of hydrolising sites on the middle lamella per kg f.w. apple tissue
l_p	(Mm)	Length of the probe used for the confined compression test
M_H	(g)	Molecular mass of hexose units
M_w	(g)	Molecular mass of water
P	(mole/kg.f.w.)	Moles of pectin residues per kg fresh weight of apple tissue
S	(mole/kg f.w.)	Moles of hydrolising sites on starch per kg fresh weight of apple tissue
t	(S)	Time
T	(K)	Temperature
W_i	(mole/kg f.w.)	Moles of water in the intercellular spaces per kg fresh weight of apple tissue
W_c	(mole/kg f.w.)	Moles of water in the cell compartment per kg fresh weight apple tissue
f_{rel}	(-)	Relative humidity
Ψ_c	(Pa)	Total water potential in the cell compartment = $\Psi_{p,c} + \Psi_{p,c}$
Ψ_i	(Pa)	Total water potential in the intercellular space compartment
y_∞	(Pa)	Total water potential of the ambient = f(T, f_{rel} & others)
Ψ_p	(Pa)	Osmotic potential: $\Psi_{p,c}$ in the cell , $\Psi_{p,i}$ in the intercellular space
$\Psi_{p,c}$	(Pa)	Turgor pressure in the cell compartment

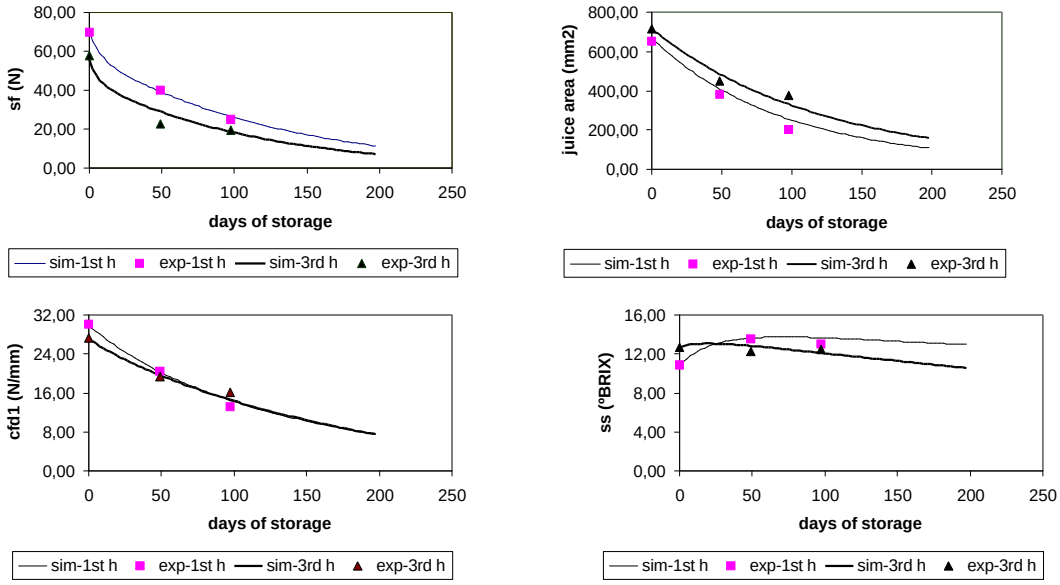

Figure 2. Experimental vs. fitted data for early (1st h) and late (3rd h) harvested, big size, *Golden* apples. Initial and model parameters' values are indicated in Table 5.

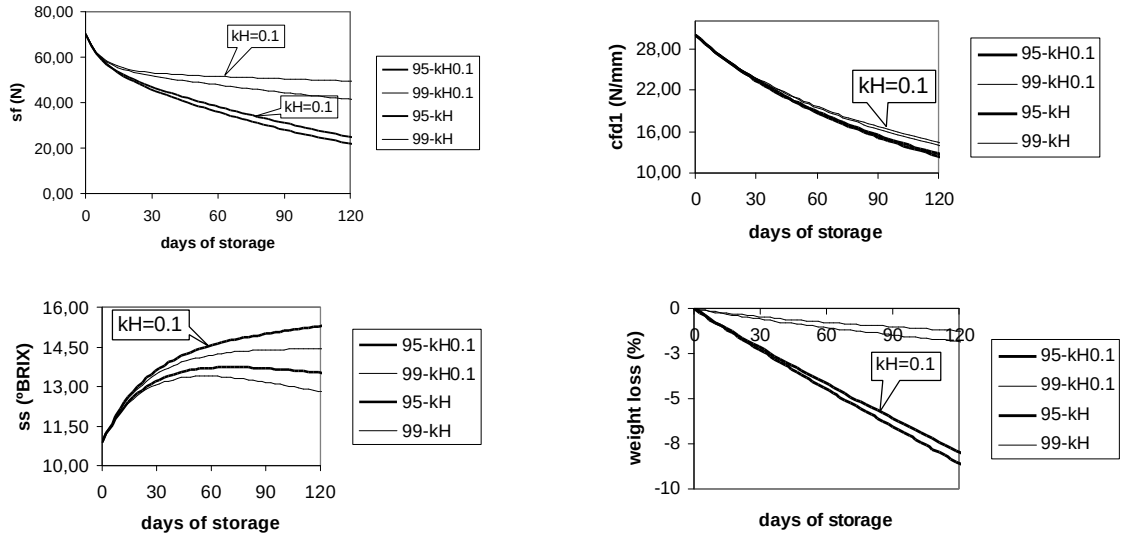

Figure 3. Kinetics of early harvested, big size, *Golden* apples for several humidity conditions (95 & 99RH) and respiration rates (0.1 k_H & k_H).

Table 5. Manually fitted values for state variables and model parameters. Experimental data correspond to early (1) and late (3) harvested, big size, *Golden* apples.

Initial Values		Early Harvest			Late Harvest
S_0	[mole/kg.fr.wt]	1.5e-01			3.89e-02
H_0	[mole/kg.fr.wt]	4.84e-01			5.58e-01
L_0	[mole/kg.fr.wt]	2.06e-02			1.84e-02
P_0	[mole/kg.fr.wt]	3.04e-03			6.17e-04
W_{c0}	[mole/kg.fr.wt]	4.45e+01			4.39e+01
W_{i0}	[mole/kg.fr.wt]	2.68e+00			1.86e+00
Model Parameters: Early Harvest (left) and Late Harvest (right)					
k_S	[1/s]	4.63e-07	a	[Pa]	9.33e+06
k_H	[1/s]	1.39e-08 ; 2.31e-08	b	[N/√m]	3.00e+01
k_L)	[1/s]	1.22e-07 ; 5.79e-08	c	[mm^2 kg.fr.wt./mole]	1.61e+01
h_mA_c	[mole/Pa s]	3.47e-12	d	[-]	2.63e+00
$h_{mi}A_i$	[mole/Pa s]	6.94e-14	e	[m^2]	3.00e-06
N_c	[1/kg.fr.wt]	6.60e+07	f	[-]	6.77e-01
E_o	[N/m^2]	1.00+05	g	[N kg.fr.wt./m^2 mole]	8.80e+07