Software tools for modelling temperature dependence of isotherms and transient water activity in selected materials

Workshop on Metrology for Humidity
at High Temperatures and non-static Conditions

Nov. 16/17, 2017 - Physikalisch-Technische Bundesanstalt, Braunschweig

The EMPIR initiative is co-funded by the European Union's Horizon 2020 research and innovation programme and the EMPIR Participating States

Outline

- Introduction;
- Examples of 3D numerical simulations;
- Experimental analysis for the determination of isotherms in hazelnuts;
- A numerical tool for the transient moisture transport in hazelnuts;
- Set-up at DTI capable of finding SI-traceable water sorption isotherms;
- Conclusions

Introduction

- Due to the risk of mould-formation and bacterial growth, many food and feed products need to have sufficiently low water activities at room temperature before being put on the market.

- Manufacturers prefer high water content, as products sold by weight then generate higher revenue.

- Costumers prefer consistent water content for fewer changes in their process.

Low water activity

No bacterial growth -> long shelf life 🙂
Low water content -> lower sales price ☹
More energy used for drying -> bad for the environment ☹

High water activity

High bacterial growth -> short shelf life ☹
High water content -> High sales price 🙂
Less energy used for drying -> good for the environment 🙂

Introduction

- In order to determine water activity, material samples are taken from the process and measured using laboratory analysers.
  - takes place hours after production;
  - no possibility of regulating production parameters;
  - either excessive drying or rejection of the batch.

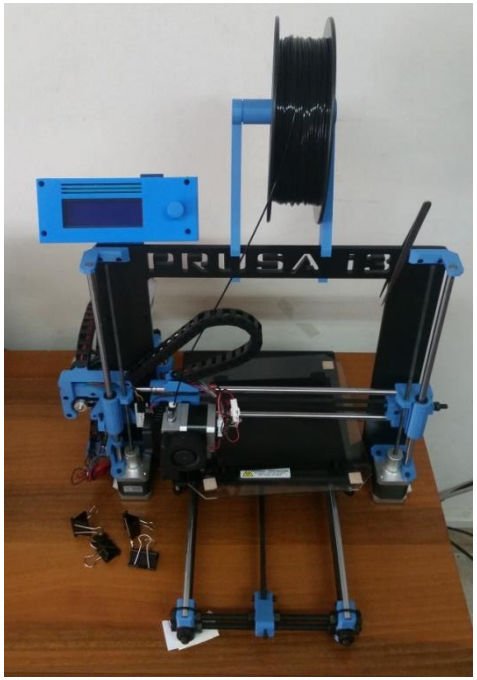
- Methods for determining water activity by in-line measurement in industry would be vital for improving cost efficiency and product quality in food and feed processing.

- Food companies allocate significant resources in order to maintain high quality monitoring of humidity in their production premises and storage facilities.

- The significant developments of Computational Fluid Dynamic technique in the last years made this tool of investigation a valid support to experiments, allowing a significant reduction of tests' times and costs.

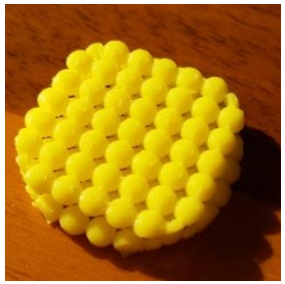
- The transient behavior of moisture-related phenomena and the influence of surface moisture and moisture transport/diffusion on the measuring instruments and techniques requires a detailed knowledge of temperature, pressure, velocity and species concentration in the physical domain under investigation (e.g. at the surface, in the bulk, at the boundary layer).

Relative humidity profile determination in cylindrical porous samples

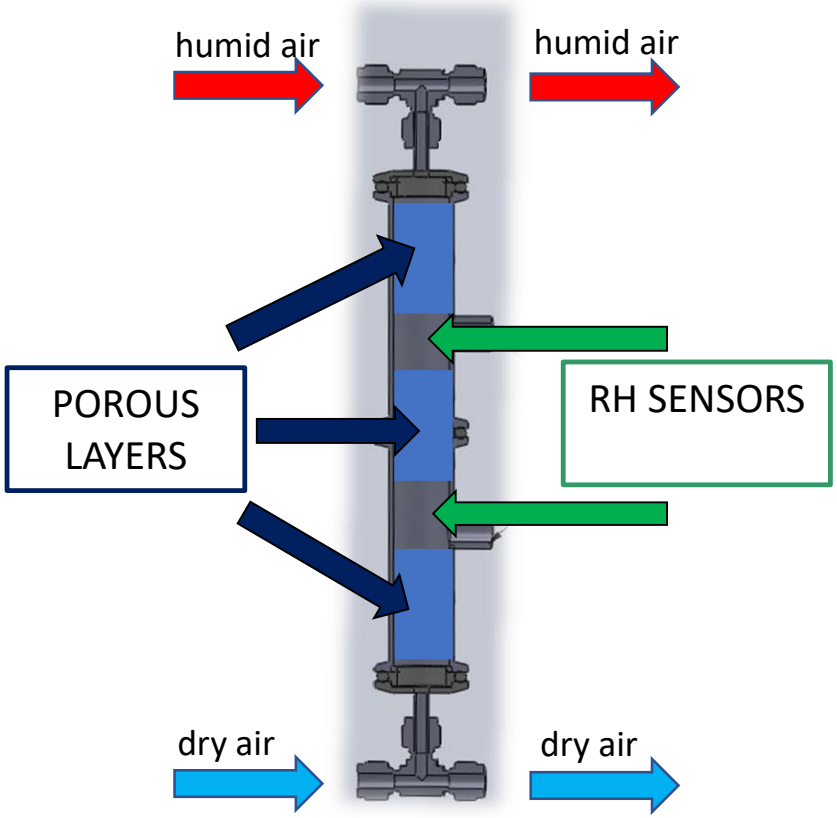


3D printer
Resolution=50 µm

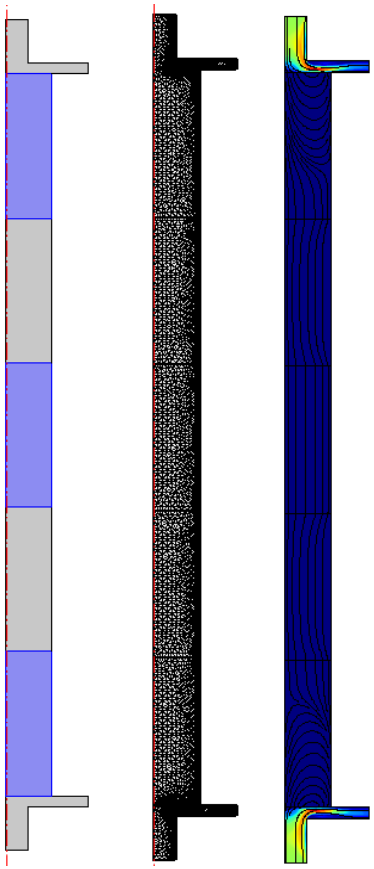
Plane of spheres
(D=0.5 mm)



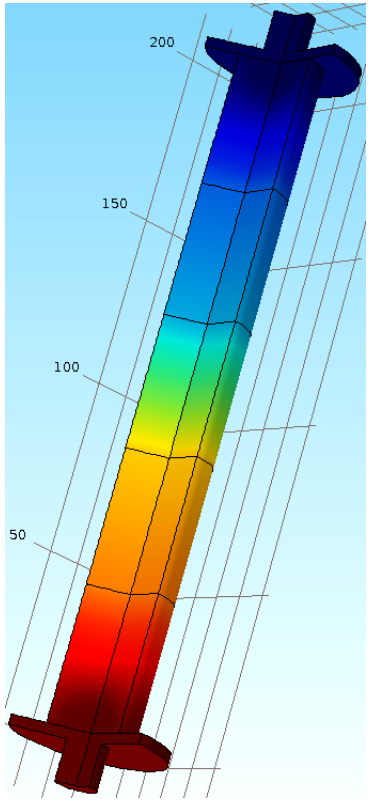
Planes of spheres (D=2 mm)



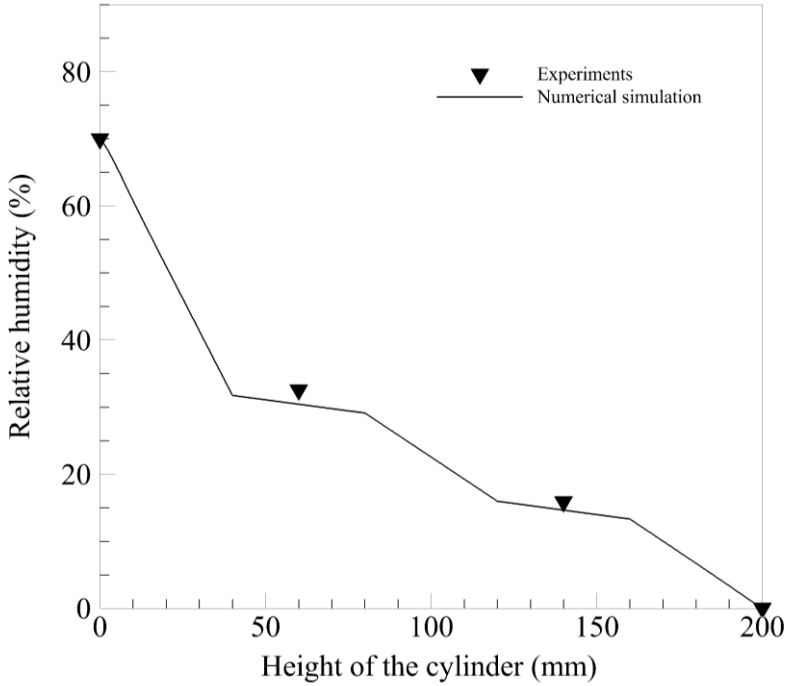
Relative humidity profile determination in cylindrical porous samples



Computational domain, used grid and veocity contour

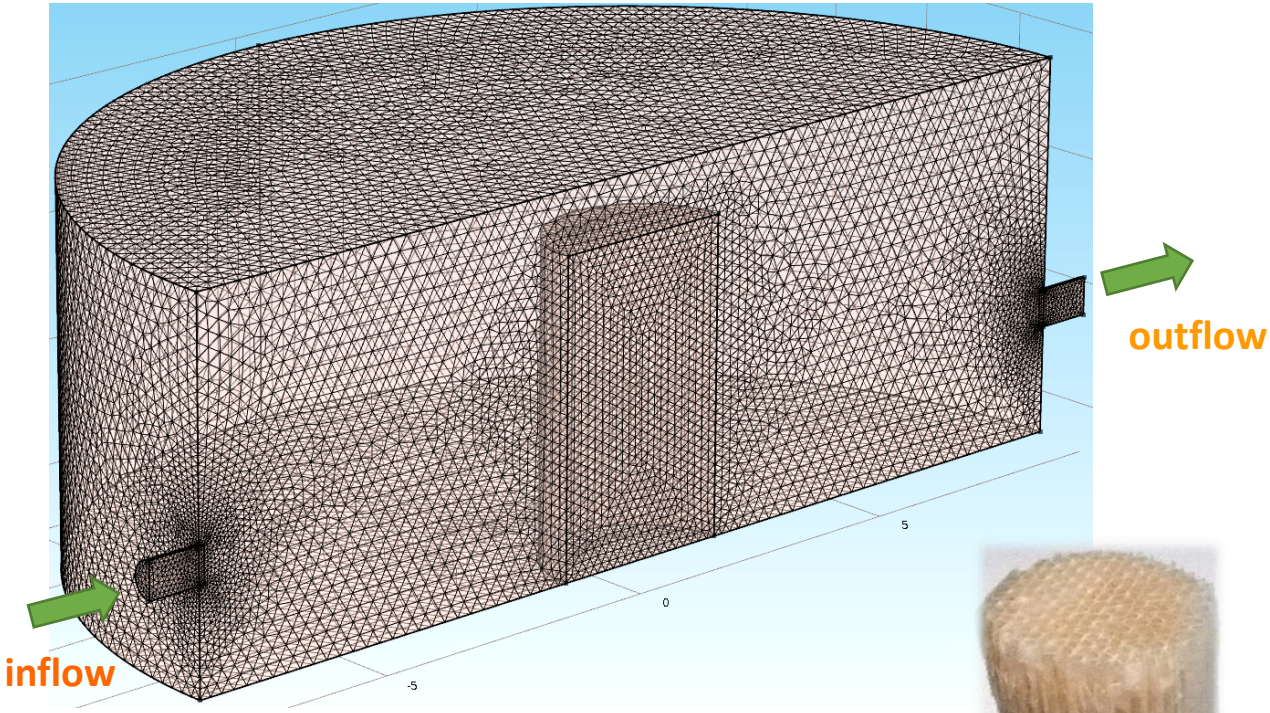


Moisture contour



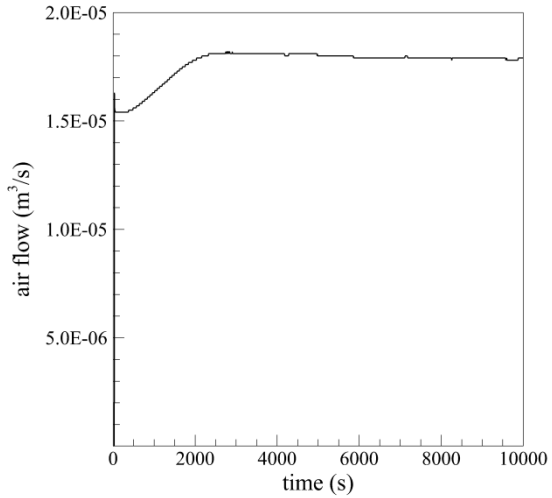
Relative humidity as a function of the z-axis

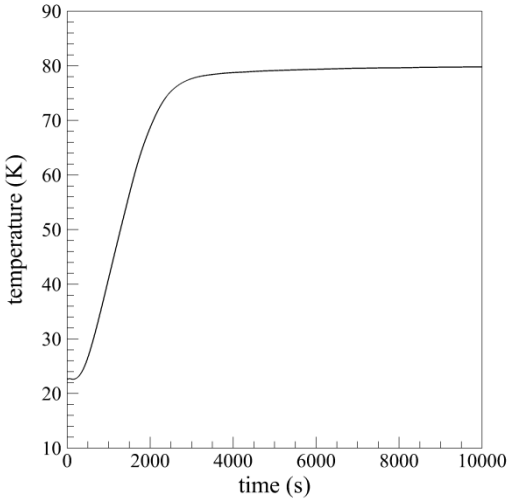
Water accumulation from a saturated porous sample



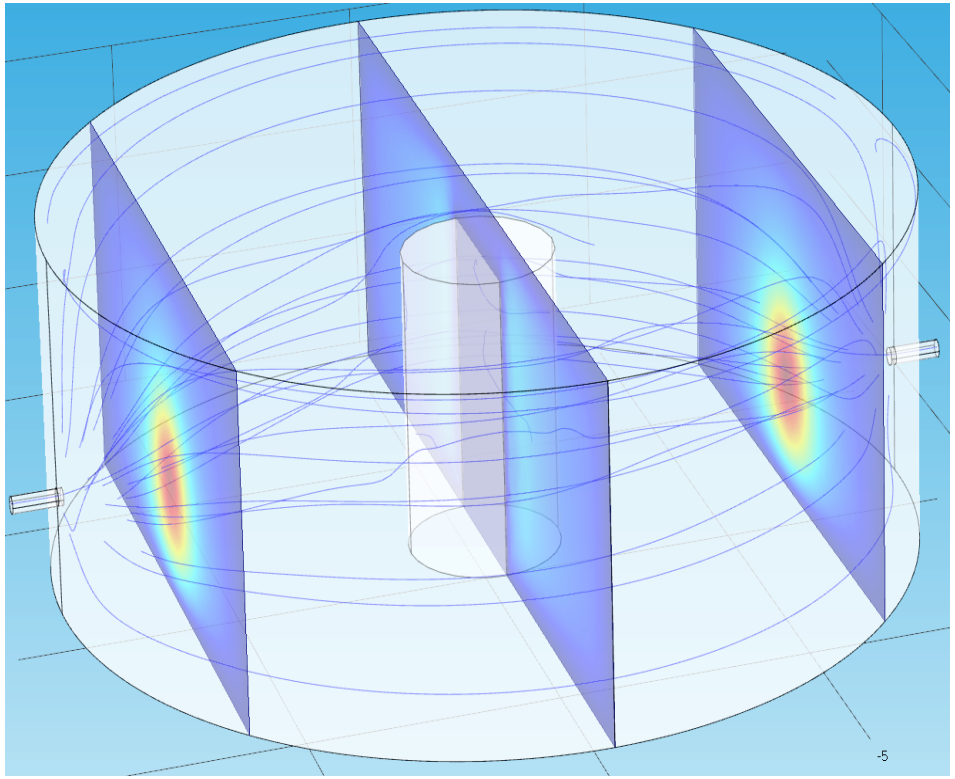
Computational domain and computational grid

porous sample
(corrugated paper + 86% of silica gel)

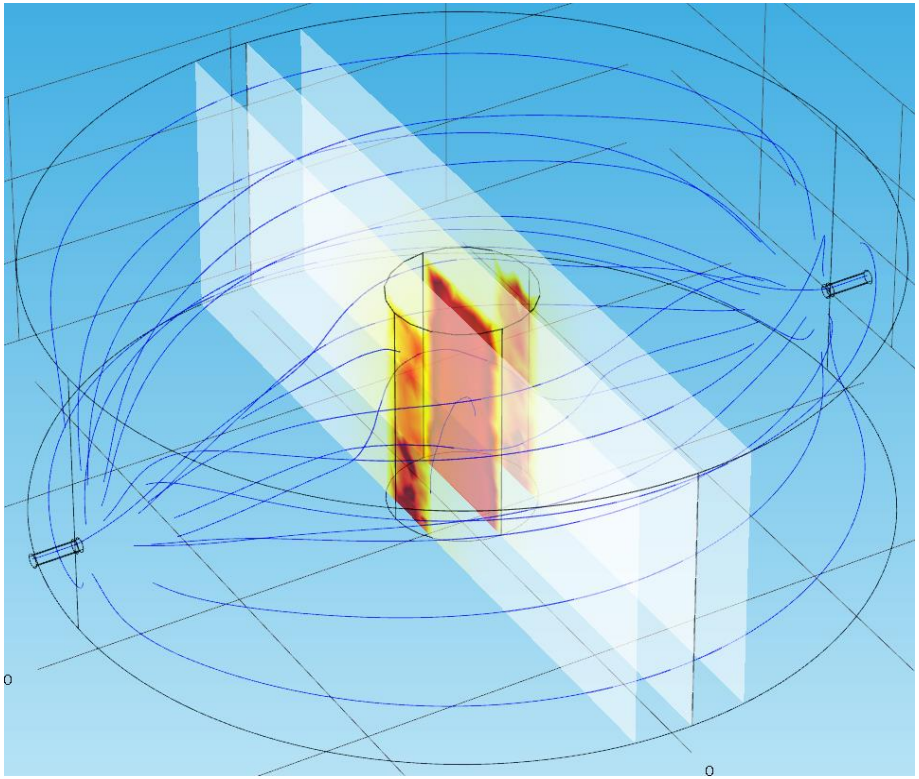




Water accumulation from a saturated porous sample

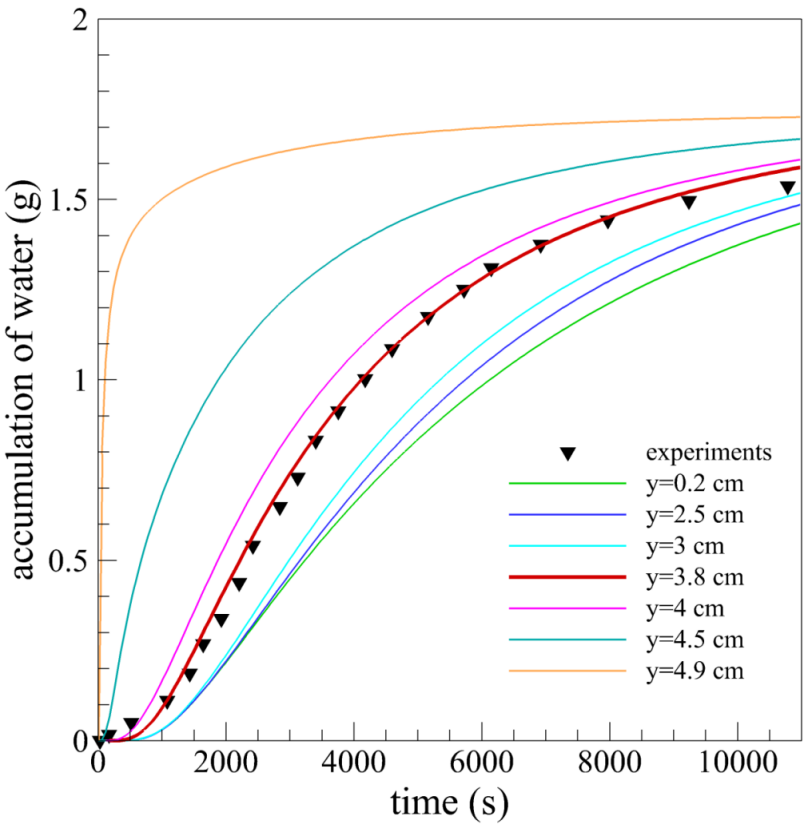


Velocity contour within the computational domain evaluated in correspondence of three different sections and a computational time of 1000s

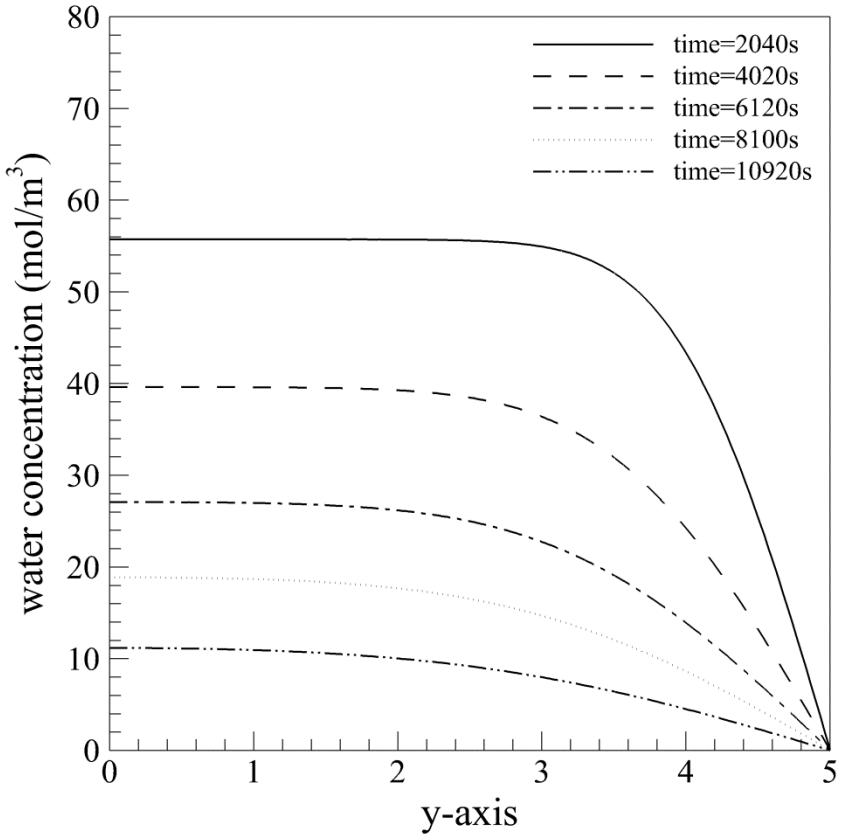


Water concentrations within the porous sample evaluated in correspondence of three different sections and a computational time of 1000s

Water accumulation from a saturated porous sample

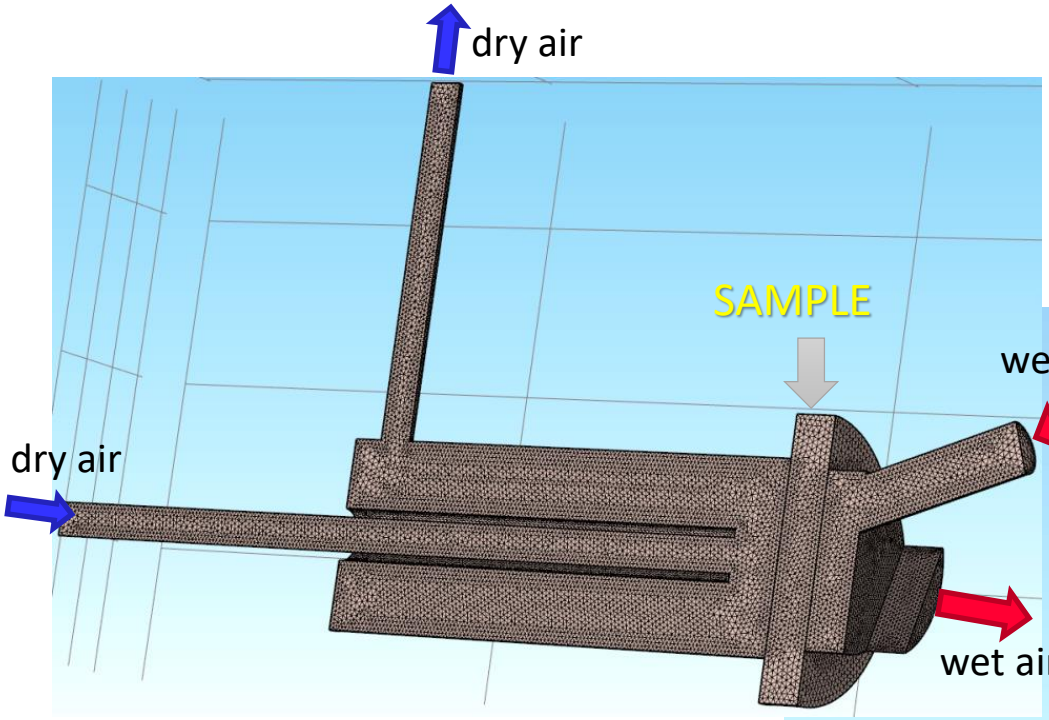


Accumulation of water as a function of time obtained in correspondence of different probes located at different heights within the sample.

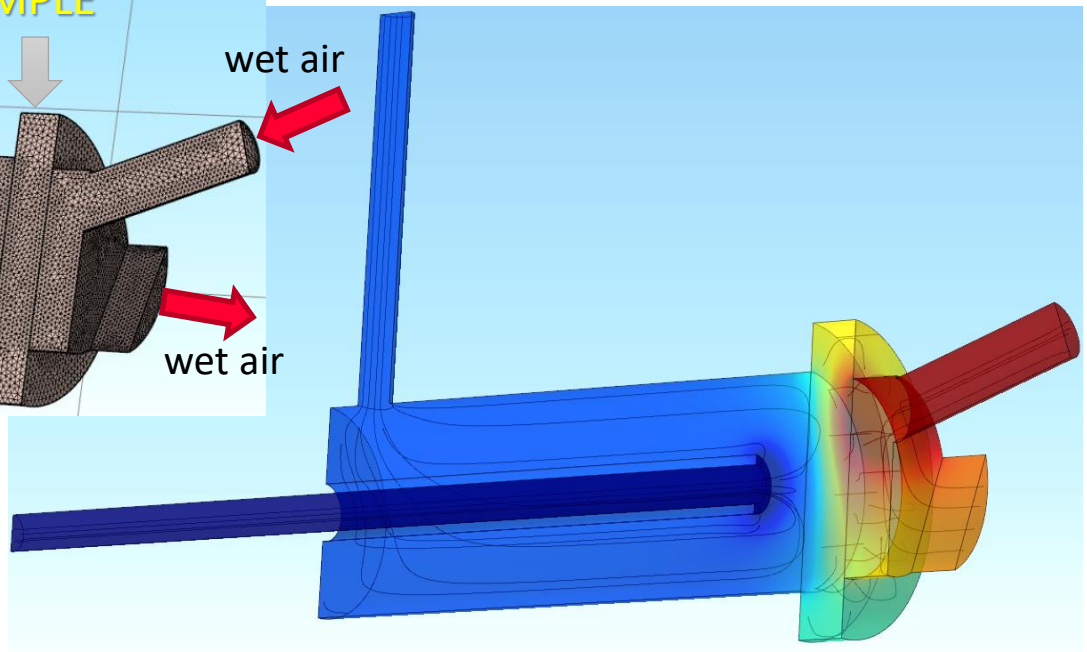


Water concentration as a function of the y-axis obtained in correspondence of different computational times.

RH distribution in a polymer located in a calibration system



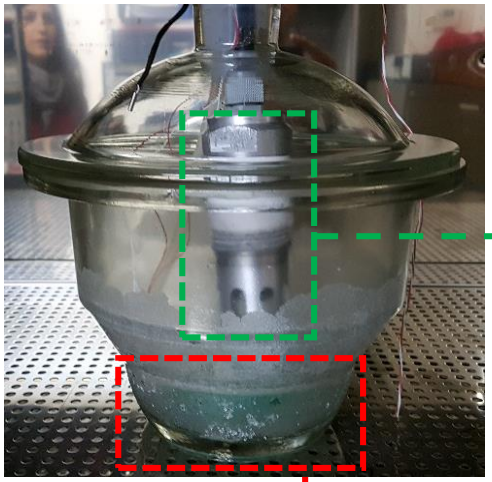
Computational domain and used grid



Qualitative moisture distribution and streamlines

Experiments on hazelnuts

- Five saturated solutions (KCH_3CO_2, K_2CO_3, KI, $(NH_4)_2SO_4$, K_2SO_4) were prepared by dissolving an appropriate quantity of salt in distilled water.

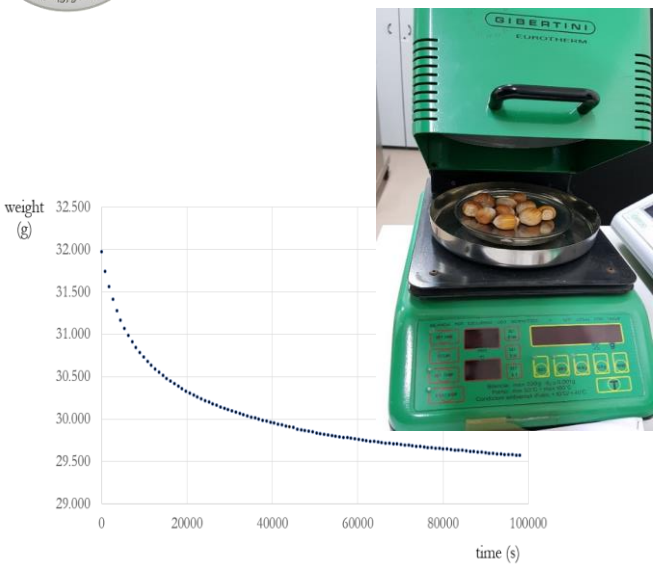


Jar containing the saturated salt solutions and 10 hazelnuts

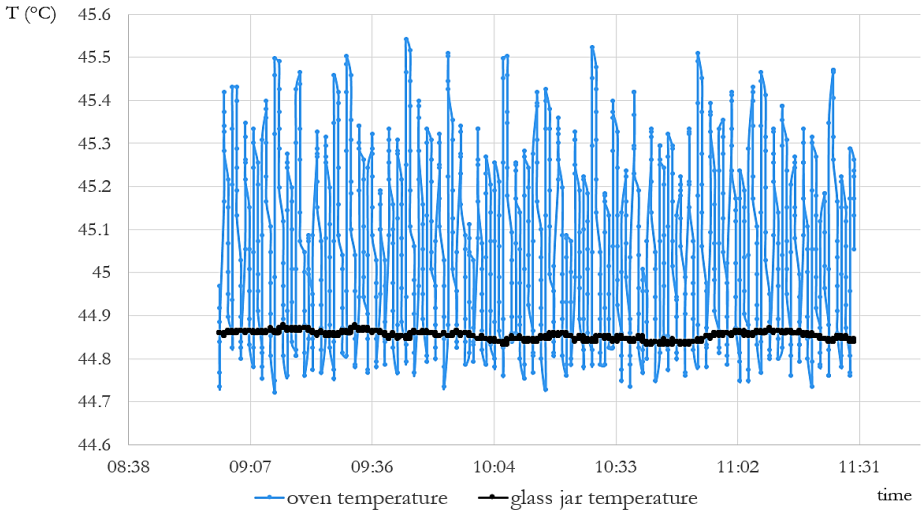
Chilled mirror dew-point hygrometer covering a dew-point range from -40 to 60 °C, with an estimated reproducibility better than 0.15 °C, and an air temperature range of -10 to +60 °C, with an estimated reproducibility better than 0.05 °C, with a coverage factor equal to 2

Hazelnuts in a plastic container

Experiments on hazelnuts



Electronic thermo-balance used to dry the hazelnuts



*Oven stability. Temperature evaluated at the centre of the oven (blue line) and temperature evaluated within the glass jar (**black line**) as a function of time*

Comparison between Relative Humidity Reference Values and Experimental Results at 20°C

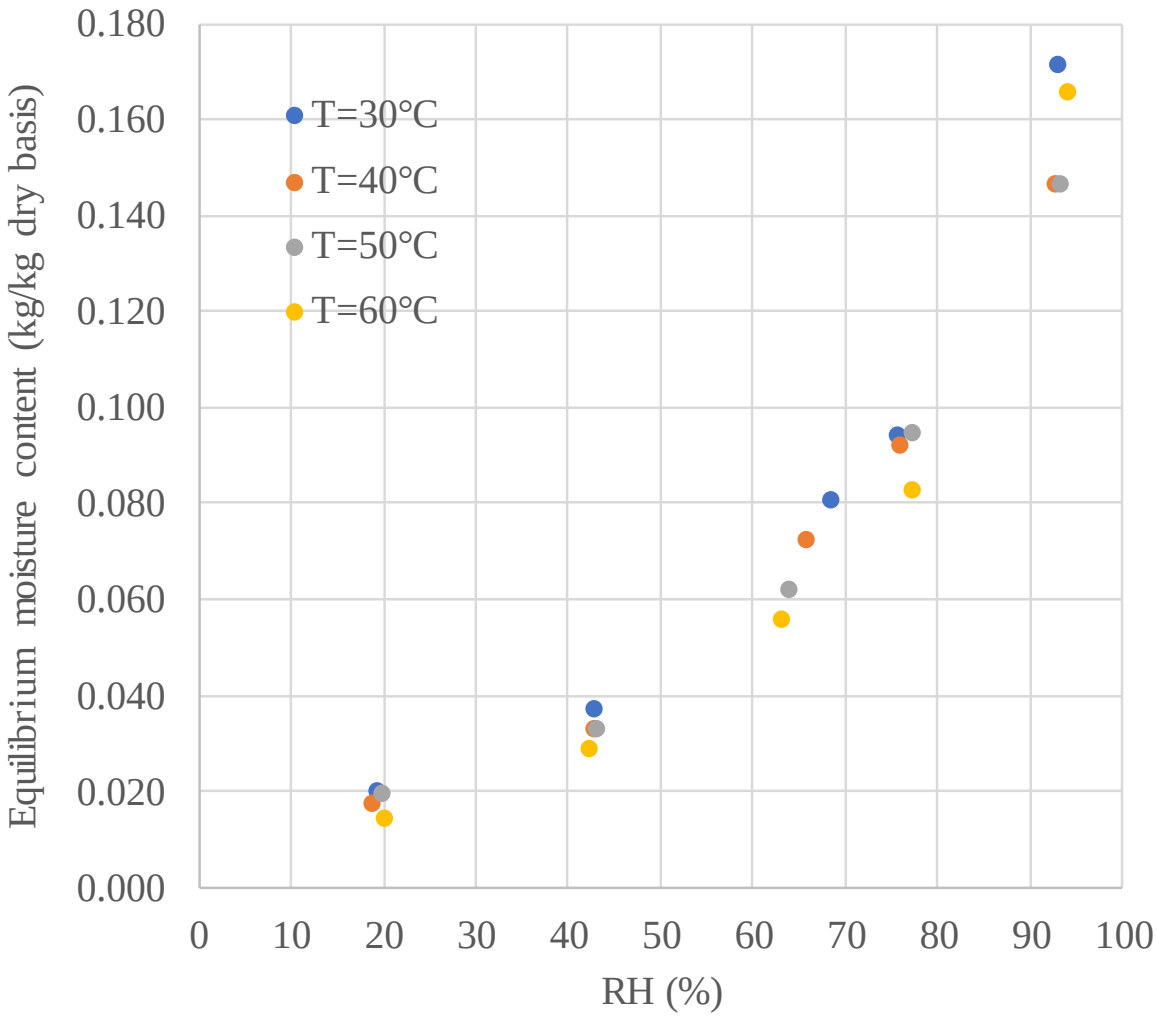
Salt	T_d result (°C)	Φ (% RH)	σ_A (% RH)	σ_B (% RH)	σ (% RH)	Greeenspan (% RH)	Wyzykowska-Szerszen (% RH)	Cretinon (% RH)
KCH_3CO_2	-1.44 ± 0.11	23.52	0.19	0.14	0.24	23.11 ± 0.25	-	-
K_2CO_3	7.21 ± 0.06	43.45	0.17	0.24	0.29	43.16 ± 0.33	-	43.9 ± 0.5
KI	14.27 ± 0.06	69.56	0.25	0.35	0.43	69.90 ± 0.26	-	-
$(NH_4)2SO_4$	16.57 ± 0.05	80.64	0.27	0.40	0.48	81.34 ± 0.31	81.3 ± 1.0	-
K_2SO_4	19.73 ± 0.06	98.33	0.38	0.48	0.62	97.59 ± 0.53	98.93 ± 1.3	-

Experiments on hazelnuts

$$X_e = \frac{m_w - m_d}{m_d}$$

m_w= mass before drying

m_d= mass after drying



Adsorption isotherms of hazelnuts obtained for a temperature of 30°C, 40°C, 50°C and 60°C

Experiments on hazelnuts

- The moisture equilibrium adsorption isotherm data obtained by experiments have been fitted to the Hailwood and Horrobin model equation reported in the following:

Hailwood and Horrobin equation

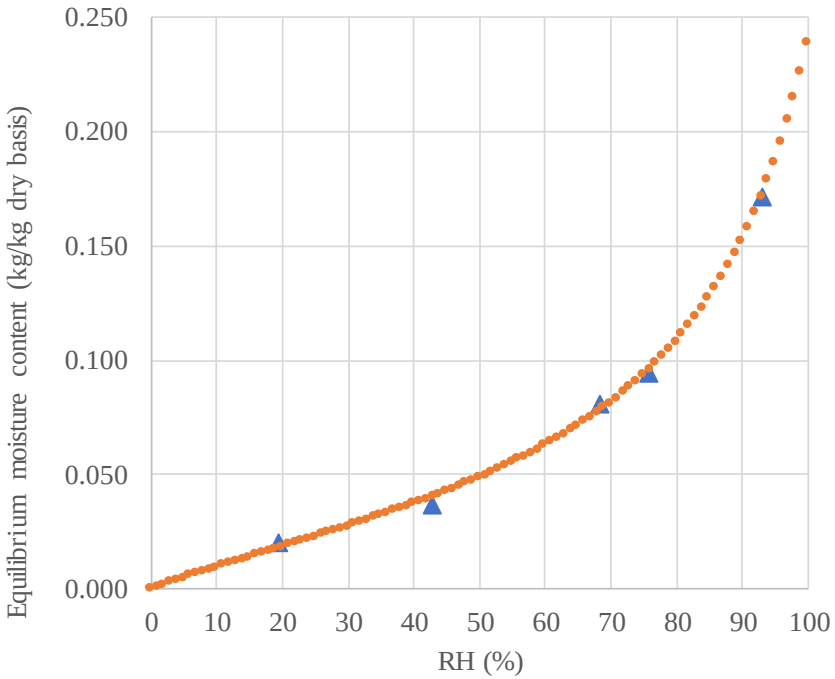
$$X_e = \frac{RH}{A + B \cdot RH - C \cdot RH^2}$$

where X_e (g) is the equilibrium moisture content and RH (%) is the relative humidity.

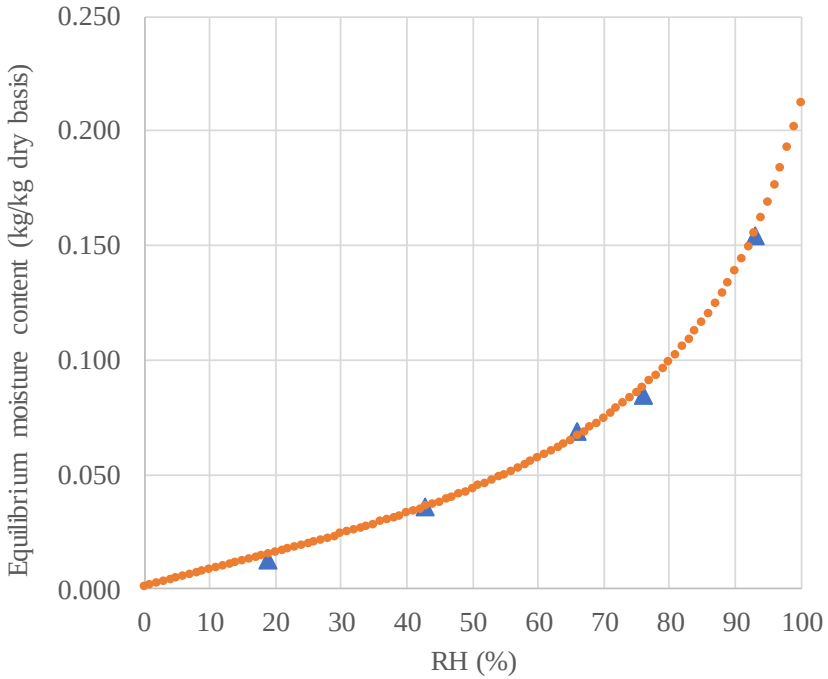
	A	B	C
T=30°C	10.035	0.069	0.001
T=40°C	13.297	0.020	0.001
T=50°C	12.994	0.046	0.001
T=60°C	12.729	0.074	0.002

Curve fitting parameters found for experimental data at different temperatures to express sorption isotherms for hazelnutz by the Hailwood and Robbin model

Experiments on hazelnuts

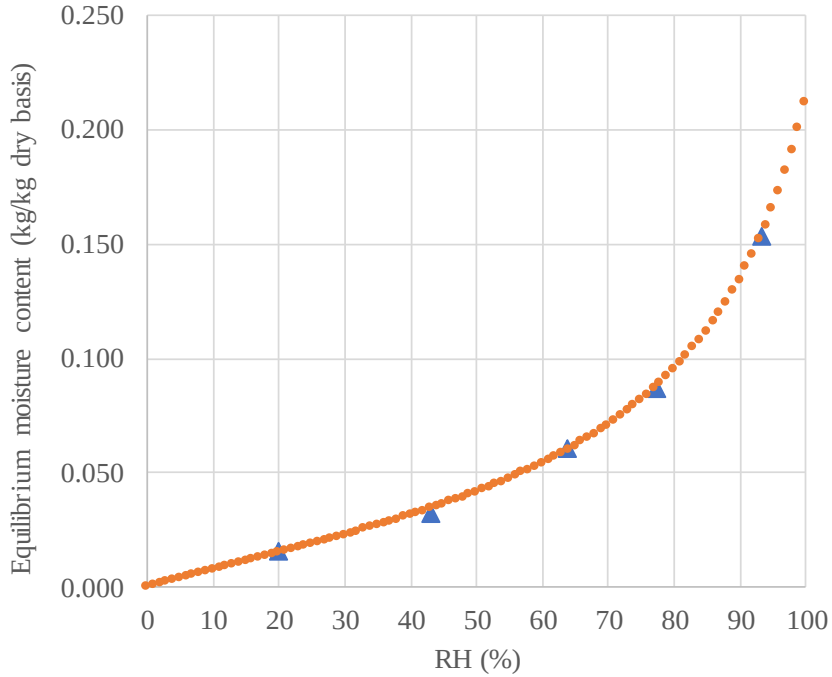


*Comparison between experimental and calculated (Hailwood and Robbin model) data of adsorption isotherms of hazelnuts obtained at **30°C***

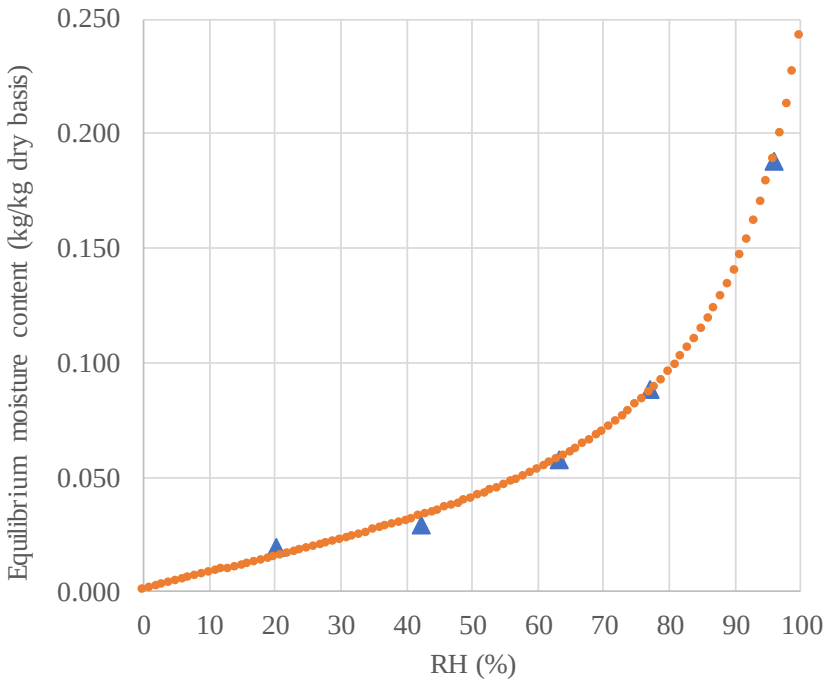


*Comparison between experimental and calculated (Hailwood and Robbin model) data of adsorption isotherms of hazelnuts obtained at **40°C***

Experiments on hazelnuts

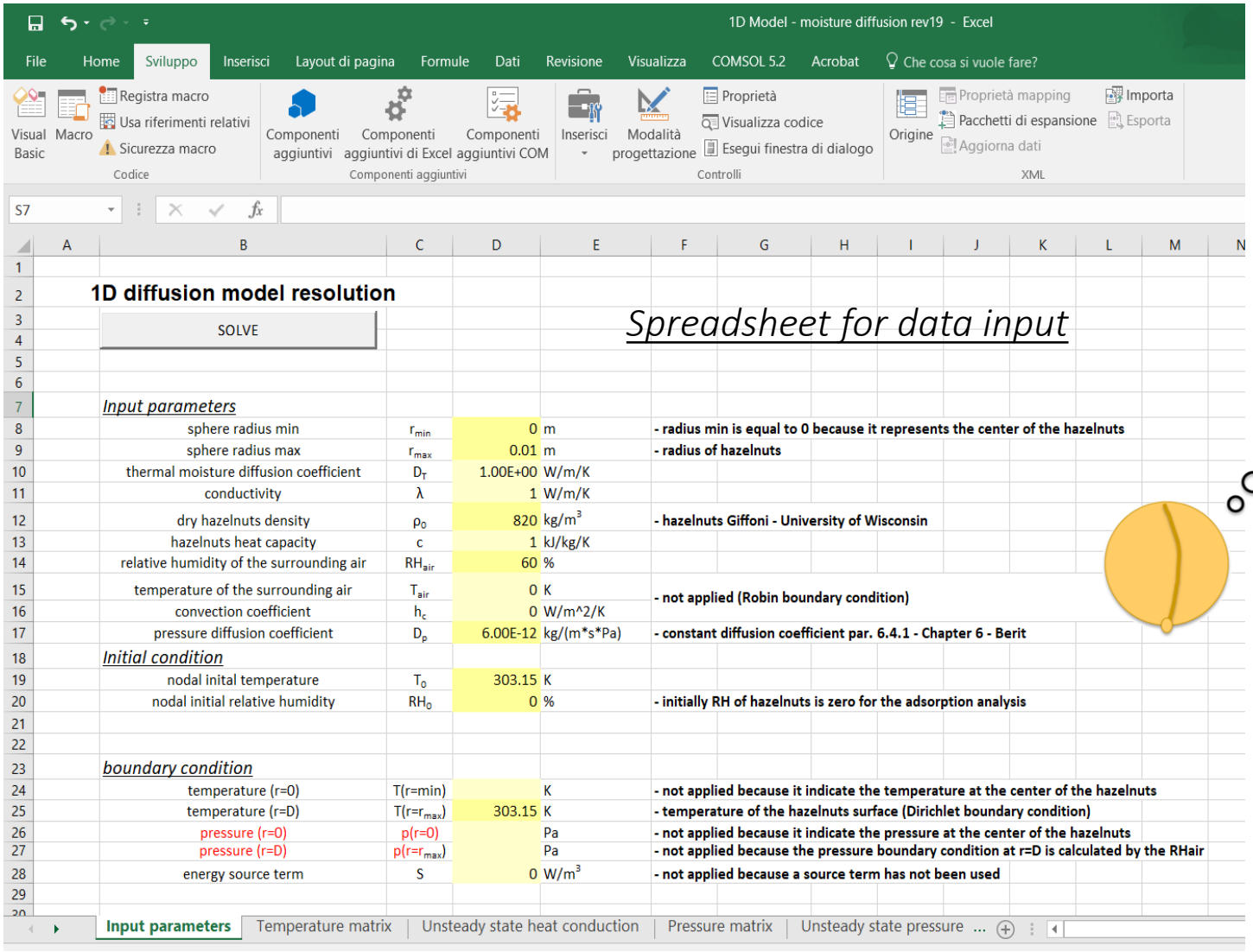


*Comparison between experimental and calculated (Hailwood and Robbin model) data of adsorption isotherms of hazelnuts obtained at **50°C***



*Comparison between experimental and calculated (Hailwood and Robbin model) data of adsorption isotherms of hazelnuts obtained at **60°C***

Numerical tool for transient moisture transport in hazelnuts



Hi, I'm a hazelnut!

Numerical tool for transient moisture transport in hazelnuts

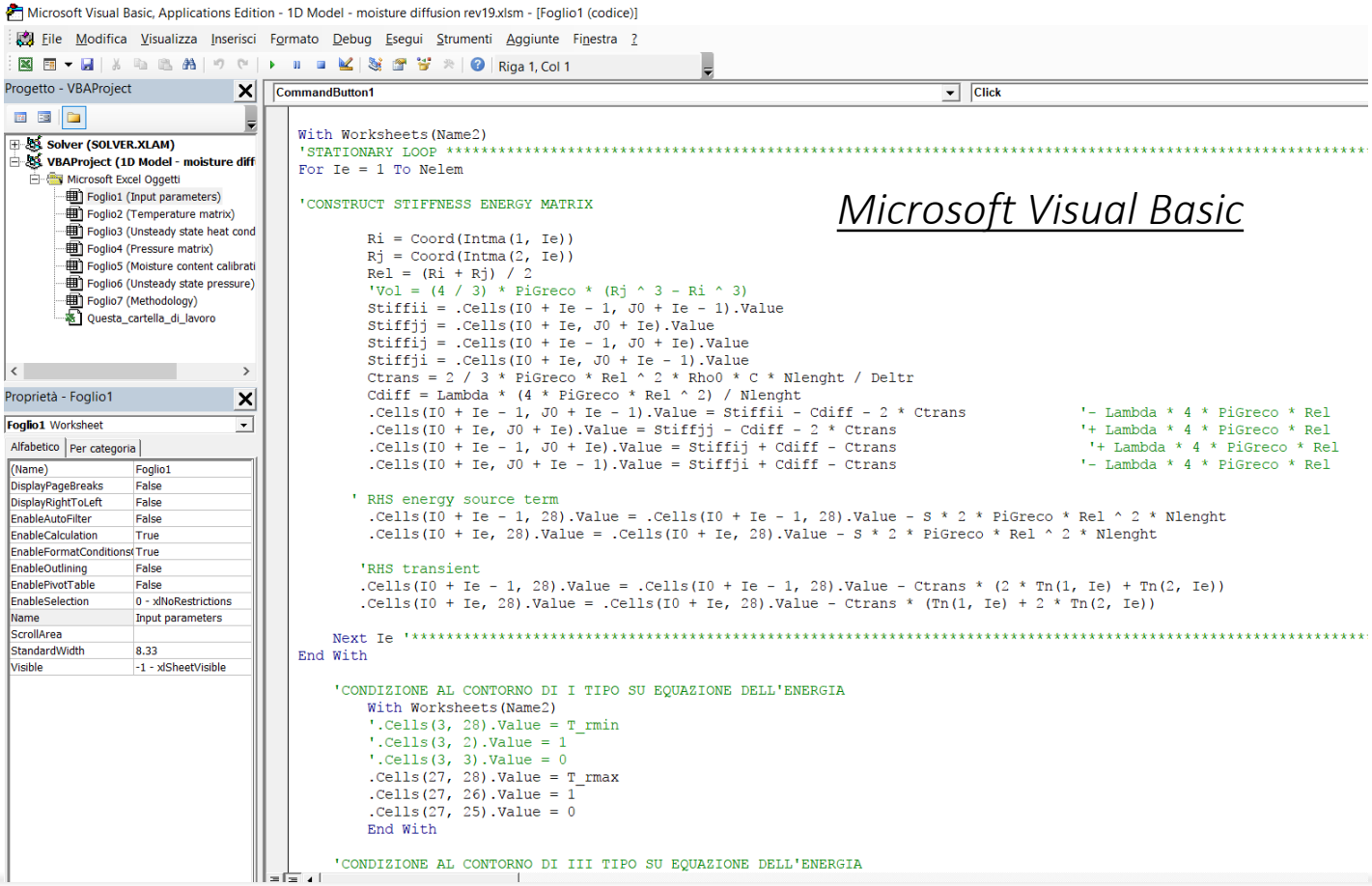
Equation for moisture

$$\left(\frac{\rho_0}{p_s^2}\frac{\partial u}{\partial \varphi}\right)\frac{\partial p}{\partial t} = D_p\frac{\partial^2 p}{\partial r^2} + D_T\frac{\partial^2 T}{\partial r^2}$$

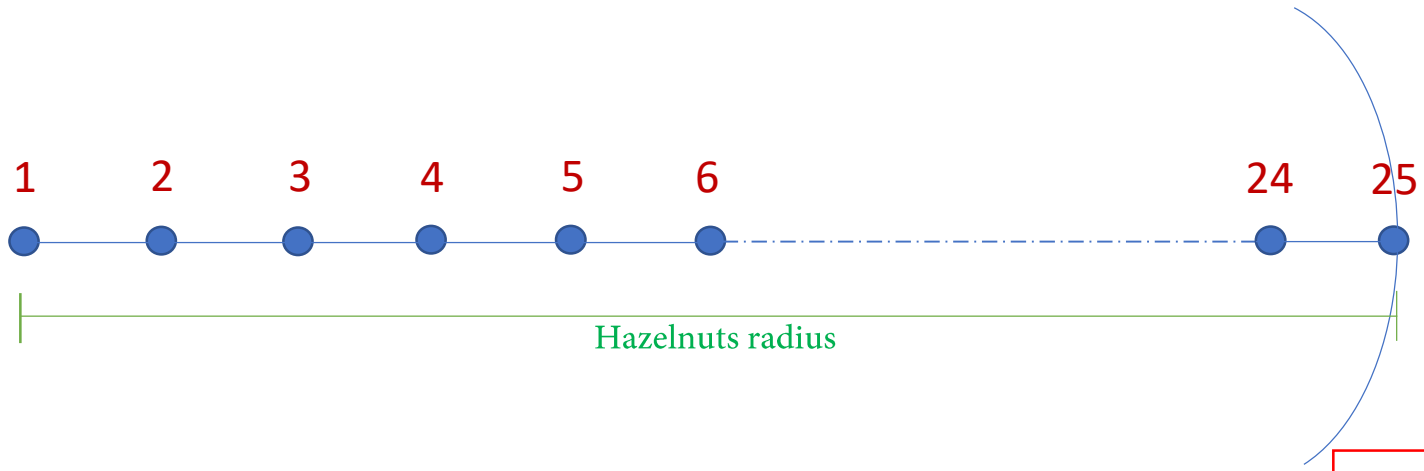
$$\varphi = \frac{p}{p_s(T)}$$

Energy conservation equation

$$\frac{\partial T}{\partial t} = \alpha\frac{\partial^2 T}{\partial r^2}\ , \qquad \alpha = \frac{\lambda}{c\rho_0}$$



Numerical tool for transient moisture transport in hazelnuts



right-hand side

Matrix assembly for the resolution of equation for moisture

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	
1	-7.9E-15	7.82E-15	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-2.9E-13
2	7.82E-15	-7.9E-14	7.03E-14	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-2.9E-12
3	0	7.03E-14	-2.7E-13	1.95E-13	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-9.7E-12
4	0	0	1.95E-13	-5.9E-13	3.83E-13	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-2.1E-11
5	0	0	0	3.83E-13	-1E-12	6.33E-13	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-3.7E-11
6	0	0	0	0	6.33E-13	-1.6E-12	9.46E-13	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-5.8E-11
7	0	0	0	0	0	9.46E-13	-2.3E-12	1.32E-12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-8.3E-11
8	0	0	0	0	0	0	1.32E-12	-3.1E-12	1.76E-12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-1.1E-10
9	0	0	0	0	0	0	0	1.76E-12	-4.1E-12	2.26E-12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-1.5E-10
10	0	0	0	0	0	0	0	0	2.26E-12	-5.2E-12	2.82E-12	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-1.9E-10
11	0	0	0	0	0	0	0	0	0	2.82E-12	-6.4E-12	3.45E-12	0	0	0	0	0	0	0	0	0	0	0	0	0	-2.3E-10
12	0	0	0	0	0	0	0	0	0	0	3.45E-12	-7.7E-12	4.13E-12	0	0	0	0	0	0	0	0	0	0	0	0	-2.8E-10
13	0	0	0	0	0	0	0	0	0	0	0	4.13E-12	-9.2E-12	4.88E-12	0	0	0	0	0	0	0	0	0	0	0	-3.3E-10
14	0	0	0	0	0	0	0	0	0	0	0	0	4.88E-12	-1.1E-11	5.7E-12	0	0	0	0	0	0	0	0	0	0	-3.9E-10
15	0	0	0	0	0	0	0	0	0	0	0	0	0	5.7E-12	-1.2E-11	6.57E-12	0	0	0	0	0	0	0	0	0	-4.6E-10
16	0	0	0	0	0	0	0	0	0	0	0	0	0	0	6.57E-12	-1.4E-11	7.51E-12	0	0	0	0	0	0	0	0	-5.3E-10
17	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	7.51E-12	-1.6E-11	8.51E-12	0	0	0	0	0	0	0	-6E-10
18	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	8.51E-12	-1.8E-11	9.57E-12	0	0	0	0	0	0	-6.8E-10
19	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	9.57E-12	-2.1E-11	1.07E-11	0	0	0	0	0	-7.6E-10
20	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1.07E-11	-2.3E-11	1.19E-11	0	0	0	0	-8.5E-10
21	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1.19E-11	-2.5E-11	1.31E-11	0	0	0	-9.4E-10
22	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1.31E-11	-2.8E-11	1.45E-11	0	0	-1E-09
23	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1.45E-11	-3.1E-11	1.58E-11	0	-1.1E-09
24	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1.58E-11	-3.4E-11	1.73E-11	-1.3E-09
25	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	2547.309

Numerical tool for transient moisture transport in hazelnuts

$$\begin{bmatrix} ii & ij & ik \\ ji & jj & jk \\ ki & kj & kk \end{bmatrix} \cdot \begin{bmatrix} RHS_i \\ RHS_j \\ RHS_k \end{bmatrix} = \begin{bmatrix} p_i \\ p_j \\ p_k \end{bmatrix}$$

25x25 25x1 25x1

nodal vapour pressure

Inverse matrix obtained by Microsoft Excel

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	p
1	-1.5E+14	-2.4E+13	-1.1E+13	-6.2E+12	-3.9E+12	-2.6E+12	-1.9E+12	-1.3E+12	-9.9E+11	-7.4E+11	-5.6E+11	-4.3E+11	-3.3E+11	-2.5E+11	-2E+11	-1.5E+11	-1.2E+11	-9.1E+10	-6.9E+10	-5.2E+10	-3.8E+10	-2.6E+10	-1.6E+10	-7.7E+09	0.13222	2523.323
2	-2.4E+13	-2.5E+13	-1.1E+13	-6.3E+12	-4E+12	-2.7E+12	-1.9E+12	-1.4E+12	-1E+12	-7.5E+11	-5.7E+11	-4.3E+11	-3.3E+11	-2.6E+11	-2E+11	-1.5E+11	-1.2E+11	-9.2E+10	-7E+10	-5.3E+10	-3.8E+10	-2.7E+10	-1.6E+10	-7.8E+09	0.134145	2523.522
3	-1.1E+13	-1.1E+13	-1.1E+13	-6.4E+12	-4E+12	-2.7E+12	-1.9E+12	-1.4E+12	-1E+12	-7.6E+11	-5.8E+11	-4.4E+11	-3.4E+11	-2.6E+11	-2E+11	-1.6E+11	-1.2E+11	-9.4E+10	-7.2E+10	-5.4E+10	-3.9E+10	-2.7E+10	-1.7E+10	-7.9E+09	0.136528	2523.764
4	-6.2E+12	-6.3E+12	-6.4E+12	-6.5E+12	-4.1E+12	-2.8E+12	-2E+12	-1.4E+12	-1E+12	-7.8E+11	-5.9E+11	-4.5E+11	-3.5E+11	-2.7E+11	-2.1E+11	-1.6E+11	-1.3E+11	-9.6E+10	-7.4E+10	-5.5E+10	-4E+10	-2.8E+10	-1.7E+10	-8.1E+09	0.14009	2524.126
5	-3.9E+12	-4E+12	-4E+12	-4.1E+12	-4.3E+12	-2.9E+12	-2E+12	-1.5E+12	-1.1E+12	-8.1E+11	-6.1E+11	-4.7E+11	-3.6E+11	-2.8E+11	-2.2E+11	-1.7E+11	-1.3E+11	-1E+11	-7.6E+10	-5.7E+10	-4.2E+10	-2.9E+10	-1.8E+10	-8.4E+09	0.144988	2524.598
6	-2.6E+12	-2.7E+12	-2.7E+12	-2.8E+12	-2.9E+12	-3E+12	-2.1E+12	-1.5E+12	-1.1E+12	-8.5E+11	-6.4E+11	-4.9E+11	-3.8E+11	-2.9E+11	-2.3E+11	-1.7E+11	-1.4E+11	-1E+11	-7.9E+10	-6E+10	-4.3E+10	-3E+10	-1.9E+10	-8.8E+09	0.151342	2525.187
7	-1.9E+12	-1.9E+12	-1.9E+12	-2E+12	-2E+12	-2.1E+12	-2.2E+12	-1.6E+12	-1.2E+12	-8.9E+11	-6.7E+11	-5.1E+11	-4E+11	-3.1E+11	-2.4E+11	-1.8E+11	-1.4E+11	-1.1E+11	-8.4E+10	-6.3E+10	-4.6E+10	-3.2E+10	-2E+10	-9.2E+09	0.15928	2525.88
8	-1.3E+12	-1.4E+12	-1.4E+12	-1.4E+12	-1.5E+12	-1.5E+12	-1.6E+12	-1.7E+12	-1.3E+12	-9.5E+11	-7.2E+11	-5.5E+11	-4.2E+11	-3.2E+11	-2.5E+11	-1.9E+11	-1.5E+11	-1.2E+11	-8.9E+10	-6.6E+10	-4.8E+10	-3.3E+10	-2.1E+10	-9.8E+09	0.168951	2526.67
9	-9.9E+11	-1E+12	-1E+12	-1E+12	-1.1E+12	-1.1E+12	-1.2E+12	-1.3E+12	-1.4E+12	-1E+12	-7.6E+11	-5.8E+11	-4.5E+11	-3.5E+11	-2.7E+11	-2.1E+11	-1.6E+11	-1.2E+11	-9.5E+10	-7.1E+10	-5.2E+10	-3.6E+10	-2.2E+10	-1E+10	0.180536	2527.552
10	-7.4E+11	-7.5E+11	-7.6E+11	-7.8E+11	-8.1E+11	-8.5E+11	-8.9E+11	-9.5E+11	-1E+12	-1.1E+12	-8.2E+11	-6.3E+11	-4.8E+11	-3.7E+11	-2.9E+11	-2.2E+11	-1.7E+11	-1.3E+11	-1E+11	-7.6E+10	-5.6E+10	-3.8E+10	-2.4E+10	-1.1E+10	0.194248	2528.553
11	-5.6E+11	-5.7E+11	-5.8E+11	-5.9E+11	-6.1E+11	-6.4E+11	-6.7E+11	-7.2E+11	-7.6E+11	-8.2E+11	-8.9E+11	-6.8E+11	-5.2E+11	-4E+11	-3.1E+11	-2.4E+11	-1.9E+11	-1.4E+11	-1.1E+11	-8.3E+10	-6E+10	-4.2E+10	-2.6E+10	-1.2E+10	0.210342	2529.638
12	-4.3E+11	-4.3E+11	-4.4E+11	-4.5E+11	-4.7E+11	-4.9E+11	-5.1E+11	-5.5E+11	-5.8E+11	-6.3E+11	-6.8E+11	-7.4E+11	-5.7E+11	-4.4E+11	-3.4E+11	-2.6E+11	-2E+11	-1.6E+11	-1.2E+11	-9E+10	-6.6E+10	-4.5E+10	-2.8E+10	-1.3E+10	0.22912	2530.813
13	-3.3E+11	-3.3E+11	-3.4E+11	-3.5E+11	-3.6E+11	-3.8E+11	-4E+11	-4.2E+11	-4.5E+11	-4.8E+11	-5.2E+11	-5.7E+11	-6.2E+11	-4.8E+11	-3.7E+11	-2.9E+11	-2.2E+11	-1.7E+11	-1.3E+11	-9.9E+10	-7.2E+10	-5E+10	-3.1E+10	-1.5E+10	0.250936	2532.04
14	-2.5E+11	-2.6E+11	-2.6E+11	-2.7E+11	-2.8E+11	-2.9E+11	-3.1E+11	-3.2E+11	-3.5E+11	-3.7E+11	-4E+11	-4.4E+11	-4.8E+11	-5.3E+11	-4.1E+11	-3.2E+11	-2.5E+11	-1.9E+11	-1.4E+11	-1.1E+11	-7.9E+10	-5.5E+10	-3.4E+10	-1.6E+10	0.276203	2533.318
15	-2E+11	-2E+11	-2E+11	-2.1E+11	-2.2E+11	-2.3E+11	-2.4E+11	-2.5E+11	-2.7E+11	-2.9E+11	-3.1E+11	-3.4E+11	-3.7E+11	-4.1E+11	-4.5E+11	-3.5E+11	-2.7E+11	-2.1E+11	-1.6E+11	-1.2E+11	-8.8E+10	-6E+10	-3.8E+10	-1.8E+10	0.305408	2534.633
16	-1.5E+11	-1.5E+11	-1.6E+11	-1.6E+11	-1.7E+11	-1.7E+11	-1.8E+11	-1.9E+11	-2.1E+11	-2.2E+11	-2.4E+11	-2.6E+11	-2.9E+11	-3.2E+11	-3.5E+11	-3.9E+11	-3E+11	-2.3E+11	-1.8E+11	-1.3E+11	-9.7E+10	-6.7E+10	-4.2E+10	-2E+10	0.339118	2535.993
17	-1.2E+11	-1.2E+11	-1.2E+11	-1.3E+11	-1.3E+11	-1.4E+11	-1.4E+11	-1.5E+11	-1.6E+11	-1.7E+11	-1.9E+11	-2E+11	-2.2E+11	-2.5E+11	-2.7E+11	-3E+11	-3.4E+11	-2.6E+11	-2E+11	-1.5E+11	-1.1E+11	-7.5E+10	-4.6E+10	-2.2E+10	0.377993	2537.386
18	-9.1E+10	-9.2E+10	-9.4E+10	-9.6E+10	-1E+11	-1E+11	-1.1E+11	-1.2E+11	-1.2E+11	-1.3E+11	-1.4E+11	-1.6E+11	-1.7E+11	-1.9E+11	-2.1E+11	-2.3E+11	-2.6E+11	-2.9E+11	-2.2E+11	-1.7E+11	-1.2E+11	-8.4E+10	-5.2E+10	-2.4E+10	0.422804	2538.76
19	-6.9E+10	-7E+10	-7.2E+10	-7.4E+10	-7.6E+10	-7.9E+10	-8.4E+10	-8.9E+10	-9.5E+10	-1E+11	-1.1E+11	-1.2E+11	-1.3E+11	-1.4E+11	-1.6E+11	-1.8E+11	-2E+11	-2.2E+11	-2.5E+11	-1.9E+11	-1.4E+11	-9.4E+10	-5.8E+10	-2.7E+10	0.474447	2540.095
20	-5.2E+10	-5.3E+10	-5.4E+10	-5.5E+10	-5.7E+10	-6E+10	-6.3E+10	-6.6E+10	-7.1E+10	-7.6E+10	-8.3E+10	-9E+10	-9.9E+10	-1.1E+11	-1.2E+11	-1.3E+11	-1.5E+11	-1.7E+11	-1.9E+11	-2.1E+11	-1.5E+11	-1.1E+11	-6.6E+10	-3.1E+10	0.533968	2541.425
21	-3.8E+10	-3.8E+10	-3.9E+10	-4E+10	-4.2E+10	-4.3E+10	-4.6E+10	-4.8E+10	-5.2E+10	-5.6E+10	-6E+10	-6.6E+10	-7.2E+10	-7.9E+10	-8.8E+10	-9.7E+10	-1.1E+11	-1.2E+11	-1.4E+11	-1.5E+11	-1.7E+11	-1.2E+11	-7.4E+10	-3.5E+10	0.602582	2542.72
22	-2.6E+10	-2.7E+10	-2.7E+10	-2.8E+10	-2.9E+10	-3E+10	-3.2E+10	-3.3E+10	-3.6E+10	-3.8E+10	-4.2E+10	-4.5E+10	-5E+10	-5.5E+10	-6E+10	-6.7E+10	-7.5E+10	-8.4E+10	-9.4E+10	-1.1E+11	-1.2E+11	-1.3E+11	-8.4E+10	-3.9E+10	0.681705	2543.959
23	-1.6E+10	-1.6E+10	-1.7E+10	-1.7E+10	-1.8E+10	-1.9E+10	-2E+10	-2.1E+10	-2.2E+10	-2.4E+10	-2.6E+10	-2.8E+10	-3.1E+10	-3.4E+10	-3.8E+10	-4.2E+10	-4.6E+10	-5.2E+10	-5.8E+10	-6.6E+10	-7.4E+10	-8.4E+10	-9.5E+10	-4.5E+10	0.772984	2545.151
24	-7.7E+09	-7.8E+09	-7.9E+09	-8.1E+09	-8.4E+09	-8.8E+09	-9.2E+09	-9.8E+09	-1E+10	-1.1E+10	-1.2E+10	-1.3E+10	-1.5E+10	-1.6E+10	-1.8E+10	-2E+10	-2.2E+10	-2.4E+10	-2.7E+10	-3.1E+10	-3.5E+10	-3.9E+10	-4.5E+10	-5.1E+10	0.878337	2546.268
25	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	2547.309

Numerical tool for transient moisture transport in hazelnuts

Vapour pressure (p)

time (s)

deltr	0	30000	60000	90000	120000	150000	180000	210000	240000	270000	300000
		1	2	3	4	5	6	7	8	9	10
1	0.00	936.49	2015.84	2603.38	2926.92	3131.33	3272.75	3376.42	3455.45	3517.37	3566.86
2	0.00	945.21	2024.82	2609.88	2931.91	3135.35	3276.08	3379.23	3457.84	3519.42	3568.63
3	0.00	955.96	2035.79	2617.82	2938.01	3140.26	3280.15	3382.67	3460.76	3521.92	3570.78
4	0.00	971.94	2051.98	2629.52	2947.00	3147.51	3286.16	3387.72	3465.06	3525.60	3573.94
5	0.00	993.76	2073.83	2645.30	2959.10	3157.26	3294.23	3394.51	3470.83	3530.54	3578.19
6	0.00	1021.81	2101.52	2665.27	2974.42	3169.59	3304.43	3403.08	3478.11	3536.75	3583.52
7	0.00	1056.45	2135.14	2689.47	2992.98	3184.51	3316.75	3413.43	3486.88	3544.24	3589.94
8	0.00	1098.13	2174.77	2717.93	3014.78	3202.02	3331.19	3425.53	3497.13	3552.97	3597.40
9	0.00	1147.32	2220.44	2750.65	3039.84	3222.11	3347.74	3439.37	3508.82	3562.91	3605.90
10	0.00	1204.64	2272.26	2787.69	3068.18	3244.81	3366.40	3454.95	3521.96	3574.07	3615.42
11	0.00	1270.72	2330.25	2829.03	3099.76	3270.06	3387.11	3472.20	3536.48	3586.37	3625.89
12	0.00	1346.35	2394.49	2874.68	3134.60	3297.84	3409.83	3491.08	3552.33	3599.76	3637.27
13	0.00	1432.38	2465.00	2924.63	3172.62	3328.08	3434.49	3511.50	3569.41	3614.16	3649.47
14	0.00	1529.81	2541.86	2978.87	3213.80	3360.72	3461.00	3533.38	3587.66	3629.49	3662.42
15	0.00	1639.81	2625.15	3037.40	3258.09	3395.67	3489.28	3556.62	3606.97	3645.66	3676.04
16	0.00	1763.68	2714.97	3100.22	3305.42	3432.85	3519.22	3581.12	3627.24	3662.58	3690.24
17	0.00	1902.89	2811.42	3167.28	3355.69	3472.12	3550.67	3606.73	3648.34	3680.11	3704.92
18	0.00	2059.08	2914.57	3238.49	3408.69	3513.24	3583.39	3633.23	3670.06	3698.09	3719.91
19	0.00	2234.12	3024.54	3313.71	3464.21	3555.97	3617.16	3660.40	3692.22	3716.35	3735.06
20	0.00	2430.18	3141.51	3392.78	3521.97	3600.03	3651.72	3688.04	3714.64	3734.74	3750.28
21	0.00	2649.64	3265.54	3475.35	3581.53	3645.01	3686.71	3715.83	3737.07	3753.05	3765.38
22	0.00	2895.20	3396.59	3560.81	3642.26	3690.34	3721.67	3743.43	3759.22	3771.06	3780.17
23	0.00	3169.91	3534.29	3648.21	3703.29	3735.38	3756.12	3770.45	3780.81	3788.56	3794.50
24	0.00	3477.21	3677.23	3735.86	3763.41	3779.26	3789.44	3796.45	3801.50	3805.27	3808.16
25	0.00	3820.96	3820.96	3820.96	3820.96	3820.96	3820.96	3820.96	3820.96	3820.96	3820.96

nodes

Transient 1D numerical simulation. Nodal vapour pressure (Pa) as a function of time obtained for established values of the air temperature and the relative humidity.

Numerical tool for transient moisture transport in hazelnuts

Relative Humidity (RH) obtained by ⇨ $RH = p/p_s(T) * 100$

time (s)

nodes	0	30000	60000	90000	120000	150000	180000	210000	240000	270000	300000
		1	2	3	4	5	6	7	8	9	10
1	0.00	22.06	47.48	61.32	68.94	73.76	77.09	79.53	81.39	82.85	84.01
2	0.00	22.26	47.69	61.47	69.06	73.85	77.17	79.60	81.45	82.90	84.06
3	0.00	22.52	47.95	61.66	69.20	73.97	77.26	79.68	81.52	82.96	84.11
4	0.00	22.89	48.33	61.94	69.41	74.14	77.40	79.80	81.62	83.04	84.18
5	0.00	23.41	48.85	62.31	69.70	74.37	77.59	79.96	81.75	83.16	84.28
6	0.00	24.07	49.50	62.78	70.06	74.66	77.83	80.16	81.92	83.31	84.41
7	0.00	24.88	50.29	63.35	70.50	75.01	78.12	80.40	82.13	83.48	84.56
8	0.00	25.87	51.23	64.02	71.01	75.42	78.46	80.69	82.37	83.69	84.73
9	0.00	27.02	52.30	64.79	71.60	75.89	78.85	81.01	82.65	83.92	84.93
10	0.00	28.37	53.52	65.66	72.27	76.43	79.29	81.38	82.96	84.18	85.16
11	0.00	29.93	54.89	66.64	73.01	77.02	79.78	81.79	83.30	84.47	85.41
12	0.00	31.71	56.40	67.71	73.83	77.68	80.32	82.23	83.67	84.79	85.67
13	0.00	33.74	58.06	68.89	74.73	78.39	80.90	82.71	84.07	85.13	85.96
14	0.00	36.03	59.87	70.17	75.70	79.16	81.52	83.23	84.50	85.49	86.27
15	0.00	38.62	61.83	71.54	76.74	79.98	82.19	83.77	84.96	85.87	86.59
16	0.00	41.54	63.95	73.02	77.86	80.86	82.89	84.35	85.44	86.27	86.92
17	0.00	44.82	66.22	74.60	79.04	81.78	83.63	84.95	85.93	86.68	87.27
18	0.00	48.50	68.65	76.28	80.29	82.75	84.40	85.58	86.45	87.11	87.62
19	0.00	52.62	71.24	78.05	81.60	83.76	85.20	86.22	86.97	87.54	87.98
20	0.00	57.24	74.00	79.91	82.96	84.80	86.01	86.87	87.50	87.97	88.34
21	0.00	62.41	76.92	81.86	84.36	85.86	86.84	87.52	88.02	88.40	88.69
22	0.00	68.19	80.00	83.87	85.79	86.92	87.66	88.17	88.55	88.82	89.04
23	0.00	74.67	83.25	85.93	87.23	87.98	88.47	88.81	89.05	89.24	89.38
24	0.00	81.90	86.61	88.00	88.64	89.02	89.26	89.42	89.54	89.63	89.70
25	0.00	90.00	90.00	90.00	90.00	90.00	90.00	90.00	90.00	90.00	90.00

Transient 1D numerical simulation. Relative Humidity (%) as a function of time obtained for established values of the air temperature and the relative humidity.

Numerical tool for transient moisture transport in hazelnuts

Moisture content (X_e) obtained by ⇨ $X_e = RH/(A + B \cdot RH - C \cdot RH^2)$

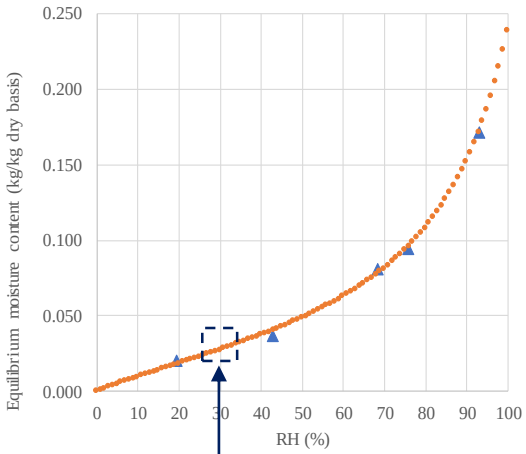
time (s)

nodes

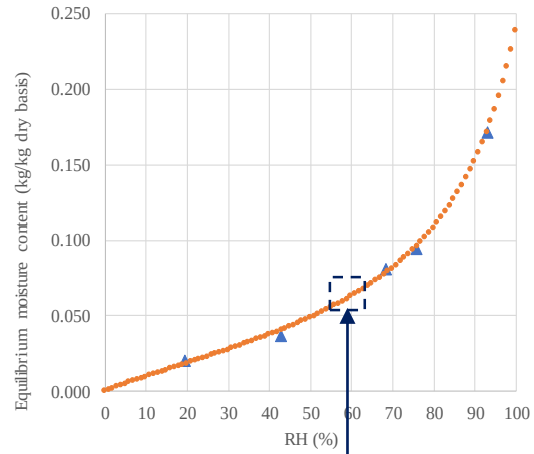
	0	30000	60000	90000	120000	150000	180000	210000	240000	270000	300000
		1	2	3	4	5	6	7	8	9	10
1	0.00000	0.00202	0.00455	0.00648	0.00790	0.00902	0.00992	0.01067	0.01131	0.01184	0.01230
2	0.00000	0.00204	0.00458	0.00651	0.00793	0.00904	0.00994	0.01069	0.01133	0.01186	0.01232
3	0.00000	0.00206	0.00461	0.00654	0.00796	0.00907	0.00997	0.01072	0.01135	0.01188	0.01234
4	0.00000	0.00209	0.00466	0.00658	0.00800	0.00911	0.01001	0.01076	0.01139	0.01192	0.01237
5	0.00000	0.00214	0.00472	0.00665	0.00807	0.00917	0.01007	0.01081	0.01144	0.01196	0.01241
6	0.00000	0.00220	0.00480	0.00673	0.00815	0.00925	0.01014	0.01088	0.01150	0.01202	0.01247
7	0.00000	0.00227	0.00490	0.00683	0.00824	0.00934	0.01023	0.01096	0.01157	0.01209	0.01253
8	0.00000	0.00236	0.00502	0.00695	0.00836	0.00945	0.01033	0.01106	0.01166	0.01217	0.01260
9	0.00000	0.00247	0.00516	0.00709	0.00849	0.00958	0.01046	0.01117	0.01177	0.01227	0.01269
10	0.00000	0.00259	0.00532	0.00725	0.00865	0.00973	0.01060	0.01130	0.01189	0.01237	0.01278
11	0.00000	0.00273	0.00551	0.00744	0.00883	0.00990	0.01075	0.01145	0.01202	0.01249	0.01289
12	0.00000	0.00290	0.00572	0.00765	0.00904	0.01010	0.01093	0.01161	0.01217	0.01263	0.01301
13	0.00000	0.00310	0.00597	0.00789	0.00927	0.01031	0.01113	0.01179	0.01233	0.01277	0.01314
14	0.00000	0.00332	0.00625	0.00817	0.00953	0.01055	0.01135	0.01199	0.01251	0.01293	0.01328
15	0.00000	0.00358	0.00657	0.00848	0.00982	0.01082	0.01159	0.01221	0.01270	0.01310	0.01343
16	0.00000	0.00389	0.00693	0.00883	0.01015	0.01112	0.01186	0.01244	0.01291	0.01328	0.01359
17	0.00000	0.00425	0.00736	0.00923	0.01052	0.01145	0.01215	0.01270	0.01313	0.01348	0.01376
18	0.00000	0.00468	0.00784	0.00969	0.01092	0.01181	0.01246	0.01297	0.01336	0.01368	0.01393
19	0.00000	0.00520	0.00841	0.01021	0.01138	0.01220	0.01280	0.01326	0.01361	0.01389	0.01411
20	0.00000	0.00584	0.00908	0.01080	0.01189	0.01263	0.01316	0.01356	0.01387	0.01411	0.01430
21	0.00000	0.00666	0.00987	0.01147	0.01245	0.01309	0.01355	0.01388	0.01414	0.01433	0.01448
22	0.00000	0.00775	0.01083	0.01225	0.01306	0.01359	0.01395	0.01421	0.01441	0.01456	0.01467
23	0.00000	0.00925	0.01200	0.01313	0.01374	0.01412	0.01437	0.01455	0.01468	0.01478	0.01486
24	0.00000	0.01149	0.01344	0.01412	0.01446	0.01466	0.01479	0.01488	0.01495	0.01500	0.01504
25	0.00000	0.01521	0.01521	0.01521	0.01521	0.01521	0.01521	0.01521	0.01521	0.01521	0.01521

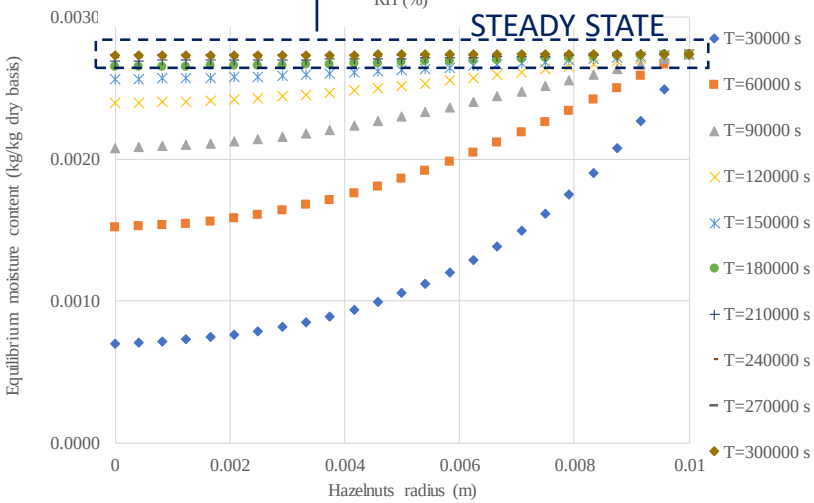
Transient 1D numerical simulation. Moisture content (kg/kg dry basis) as a function of time obtained for established values of the air temperature and the relative humidity.

Numerical tool for transient moisture transport in hazelnuts

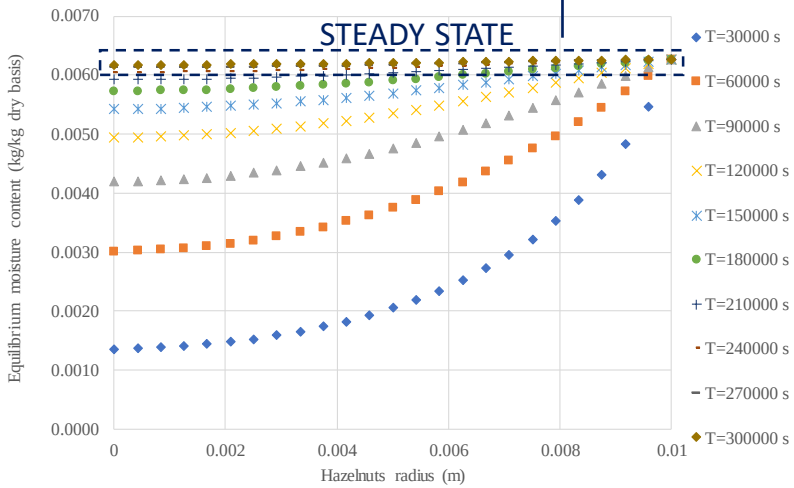


Adsorption isotherms obtained by experiments



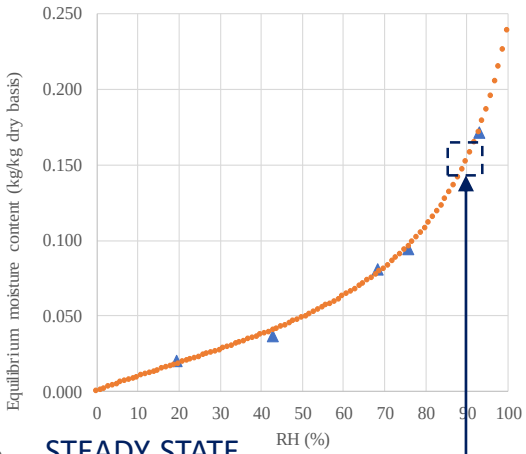


Transient 1D numerical simulation. Equilibrium moisture content as a function of the hazelnuts radius obtained in correspondence of an equilibrium ***temperature of 30°C*** *and a* ***RH=30%***

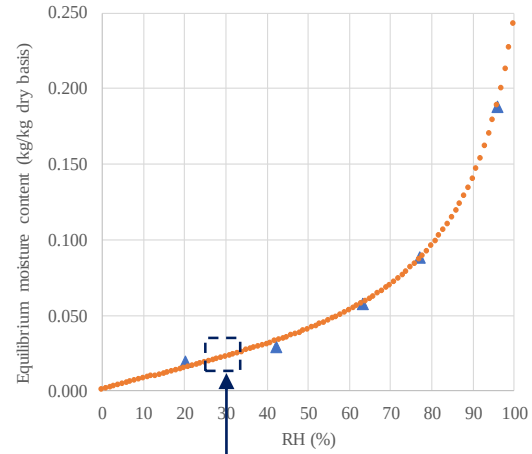


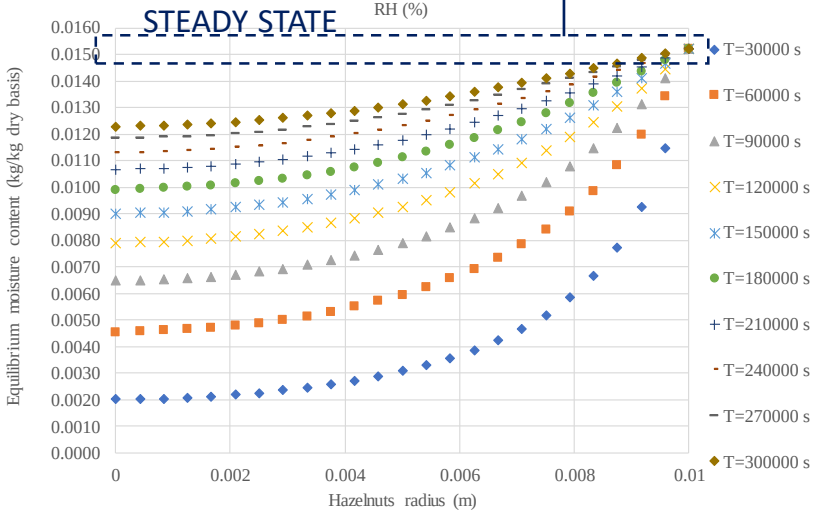
Transient 1D numerical simulation. Equilibrium moisture content as a function of the hazelnuts radius obtained in correspondence of an equilibrium ***temperature of 30°C*** *and a* ***RH=60%***

Numerical tool for transient moisture transport in hazelnuts

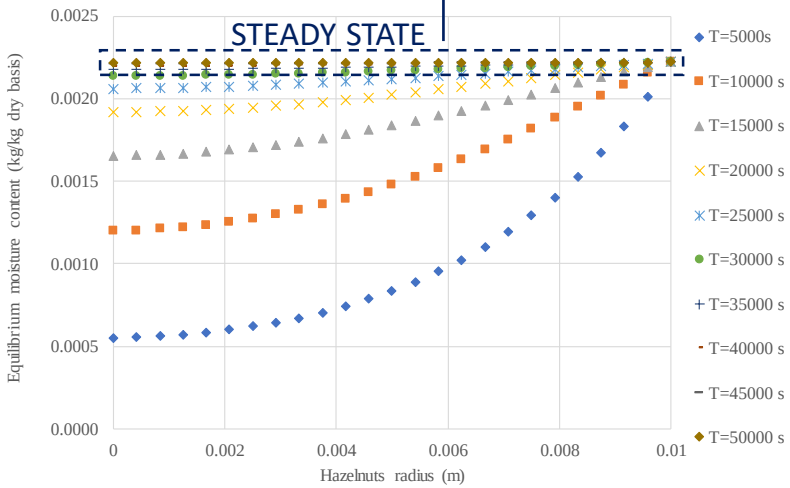


Adsorption isotherms obtained by experiments



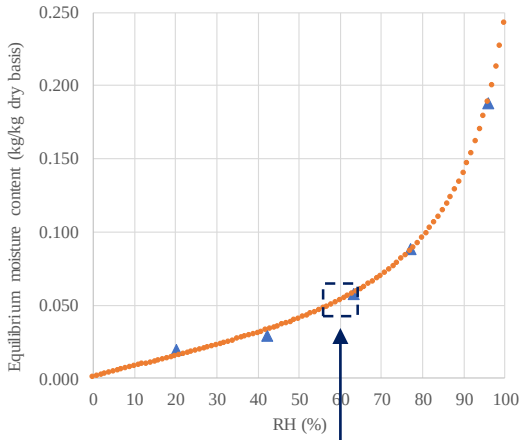


Transient 1D numerical simulation. Equilibrium moisture content as a function of the hazelnuts radius obtained in correspondence of an equilibrium ***temperature of 30°C*** *and a* ***RH=90%***

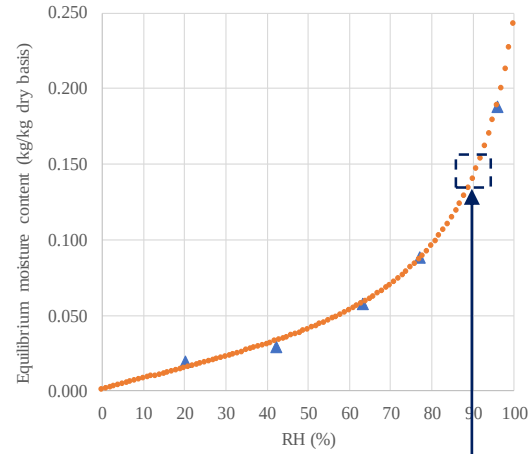


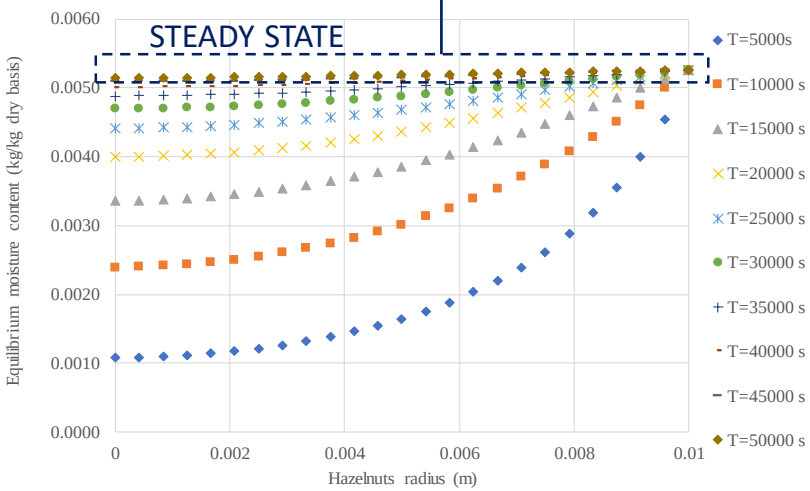
Transient 1D numerical simulation. Equilibrium moisture content as a function of the hazelnuts radius obtained in correspondence of an equilibrium ***temperature of 60°C*** *and a* ***RH=30%***

Numerical tool for transient moisture transport in hazelnuts

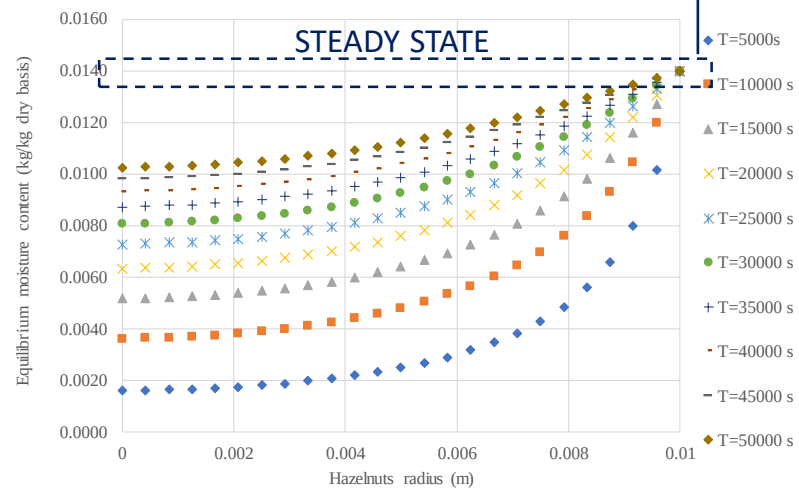


Adsorption isotherms obtained by experiments





Transient 1D numerical simulation. Equilibrium moisture content as a function of the hazelnuts radius obtained in correspondence of an equilibrium ***temperature of 60°C*** *and a* ***RH=60%***

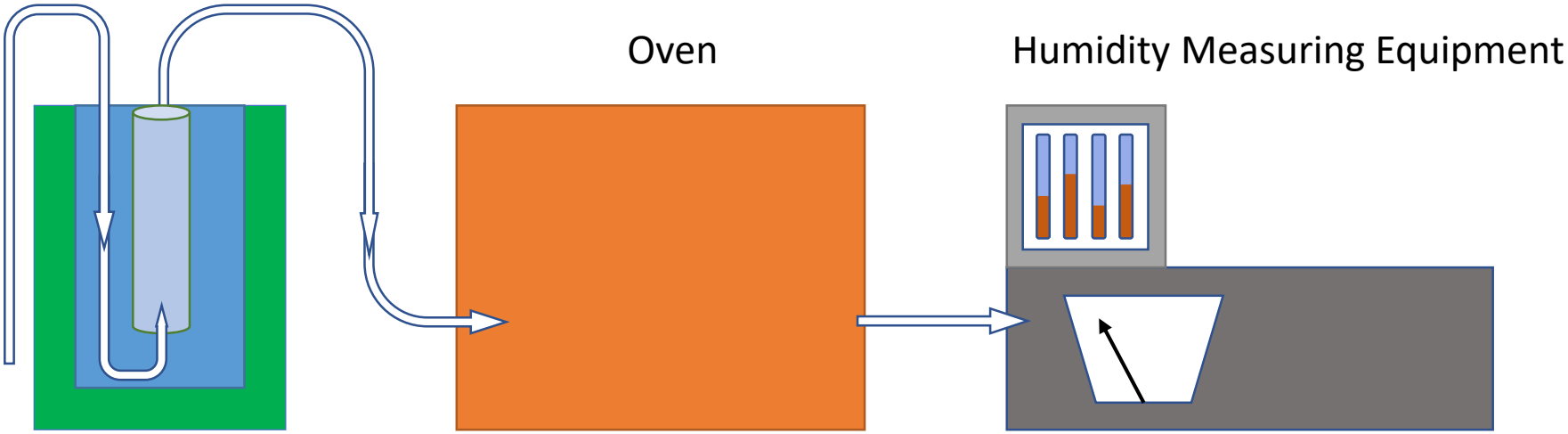


Transient 1D numerical simulation. Equilibrium moisture content as a function of the hazelnuts radius obtained in correspondence of an equilibrium ***temperature of 60°C*** *and a* ***RH=90%***

Set-up at Danish Technological Institute

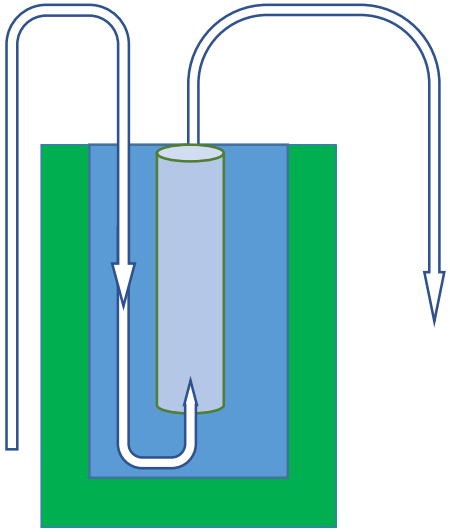
- DTI has developed a set-up, capable of finding SI-traceable water sorption isotherms.

- The setup consists of three main parts:
  - Dew point generator for making humid air;
  - Oven to heat up the humid air and the sample;
  - Humidity measuring equipment to check if the material is in equilibrium.



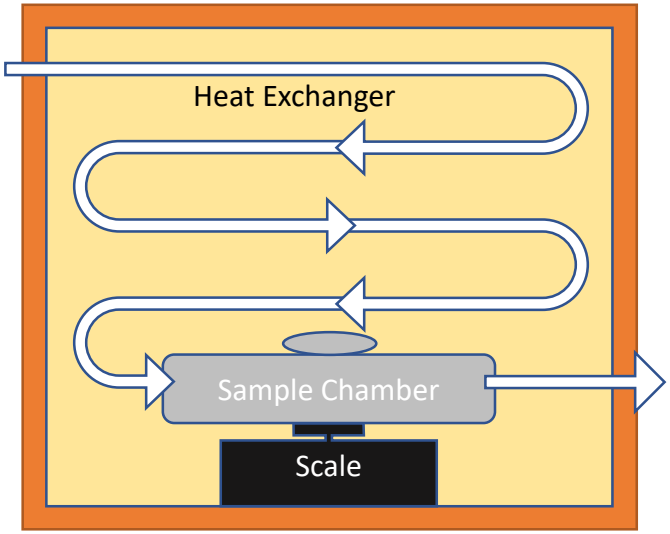
Dew Point Generator

- The Dew Point Generator consists of a water bath ($0.040\ \mathrm{m}^3$) which is temperature controlled via a cooling/heating tower (not shown in the figure).
- Air is pumped through a hose and through a filter at the bottom of a cylinder, submerged in the bath, filled with distilled water. This generates bubbles in the water filled cylinder.
- The air bubbles become saturated with water vapour, giving a gas with a dew point equal to the water bath.
- Air is transported through a heated hose to the oven.



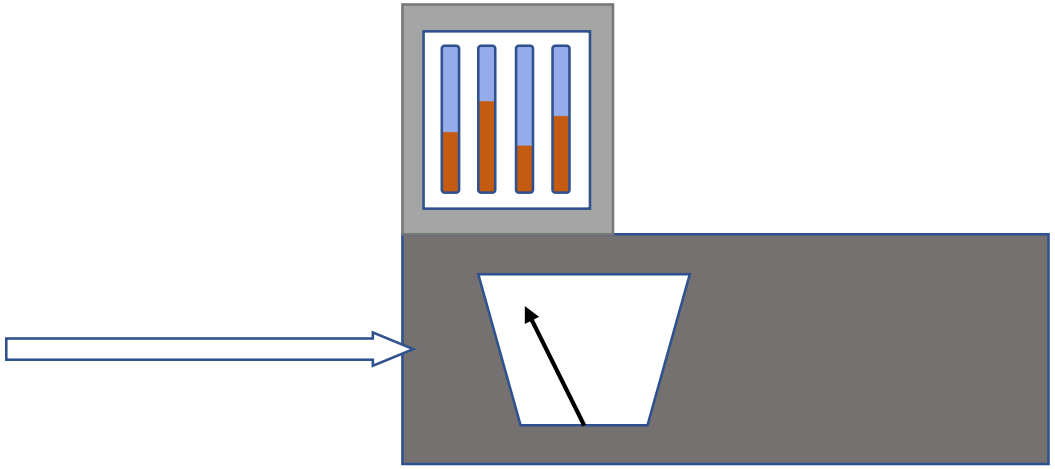
Oven

- Humid air enters the oven and is passed through a heat exchanger. This gives a known relative humidity of the gas.
- The gas is passed though the sample chamber, where the sample will either ab- or adsorb water, depending on its initial water content and temperature.
- The weight of the sample chamber is continuously measured to monitor the ab-/adsorption of water from the sample.



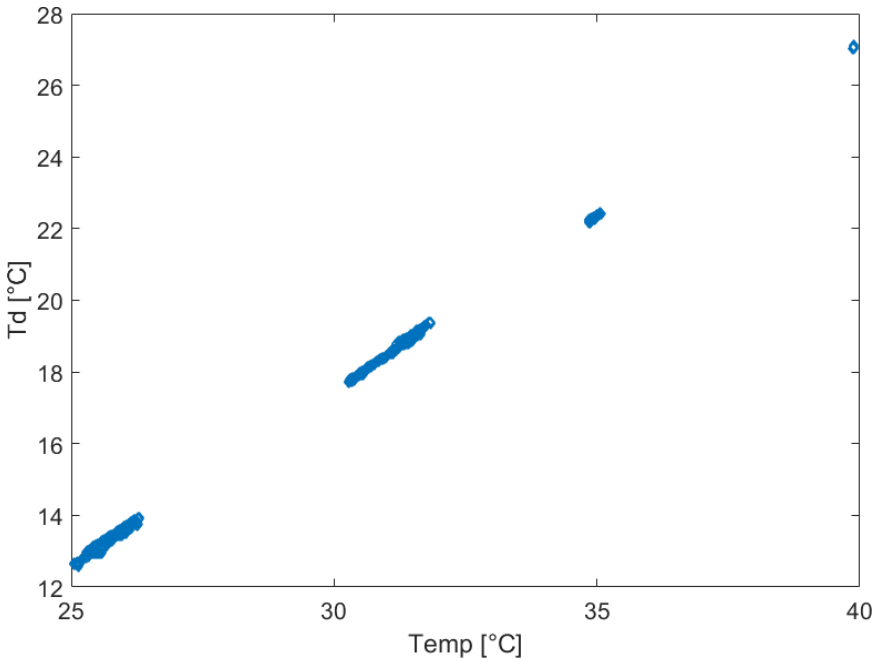
Humidity measuring equipment

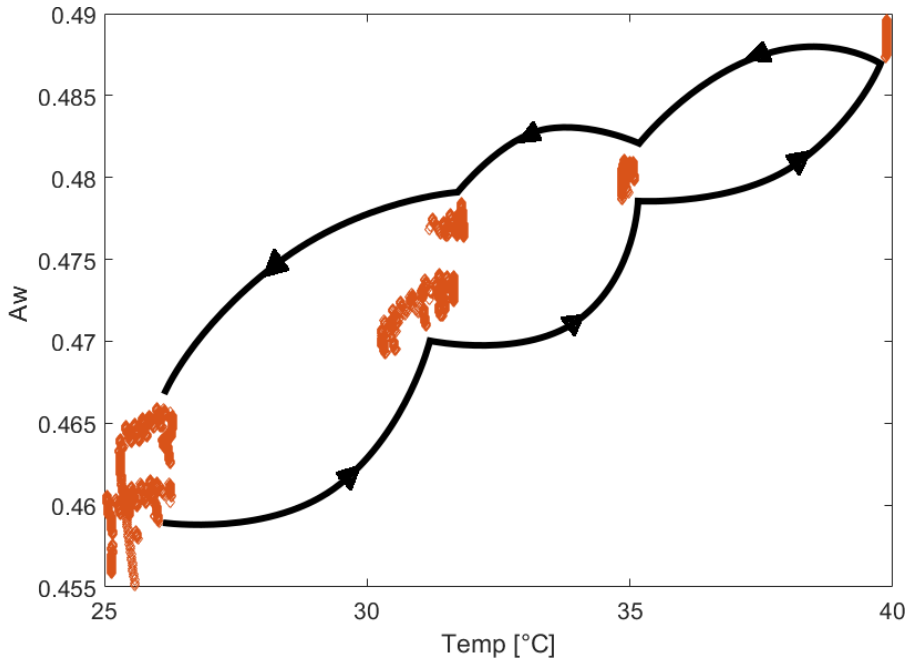
- Humidity Measuring Equipment measures both dew point of gas leaving the sample, as well as temperature of the sample.
- When the dew point of the gas leaving the sample equals the dew point of the gas entering the sample, the sample has no net-water ab-/adsorption, and is in equilibrium.
- Temperature is monitored to assure that the experiment is conducted under the correct settings.



Results

- In a setup, where the water content of the sample is kept constant (i.e. constant weight), measurements show varying water activity at different temperatures.





Conclusions

- A numerical tool for modelling the temperature dependence of sorption isotherms and transient water activity in hazelnuts has been developed.
- The model is based on Fick's law with water vapour pressure and temperature as driving potentials.
- It allows the investigation of the transient water accumulation in hazelnuts and the analysis of material properties influence on moisture sorption.
- In order to calibrate the developed numerical tool, an experimental setup has been realized for the determination of the absorption isotherms, in the temperature range of 30-60 °C.
- The experimental data of sorption in hazelnuts were fitted by the Hailwood and Horrobin equation and good results were found.
- Combining sample-based sorption isotherm measurements with the new simulation tool a novel method for traceable water activity measurements in line has been developed.
- The obtained numerical results give information about the time required for the water accumulation within the sample, at different temperature and for different relative humidity.
- Additional experimental data will allow to calibrate the numerical model also at high temperature.