Numerical Modeling and Performance Optimization Study of a Dehumidification Process in Nuclear Waste Storage

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Abstract: One of the main parameters to consider during the nuclear waste storage design phase is the drum corrosion risk. The humid-air corrosion models available in literature predict that, for carbon steel, the phenomena start to become appreciable for relative humidity (RH) values close to 65%. In general, the corrosion rate increases exponentially with relative humidity above the RH threshold. To reduce the corrosion risk an alternative technique rather than installing HVAC system is using dehumidifiers. The main objective of this study is to develop a numerical model that replicates the functioning of industrial isothermal dehumidifiers in order to obtain indications about their performance. The geometry of the rad-waste interim storage and its thermo-physical properties, considered during simulations, are taken from a specific ongoing project while the characteristic functioning curves of the dehumidifiers represent the industrial state of art.

Keywords: dehumidification, CFD, nuclear, waste-storage, corrosion.

1. Introduction

During the design phase of a nuclear waste storage the risk of corrosion of the drums plays an important role. The humid-air corrosion models available in literature predict that, for carbon steel, the phenomena start to become appreciable for relative humidity (RH) values close to 65%. In general, the corrosion rate increases exponentially with relative humidity above the RH threshold [1]. To reduce the corrosion risk an alternative technique rather than installing HVAC system is using dehumidifiers. Due to lower cost the isothermal dehumidifiers (reverse Carnot cycle) are preferred compared to rotary desiccant kind (for example silica-gel type). The main objective of this study is to develop a numerical model that replicates the functioning of industrial isothermal dehumidifiers into a storage in order to obtain indications about their performance. The geometry of the rad-waste interim storage and its thermo-physical properties, considered during simulations, are taken from a specific ongoing project while the characteristic functioning curves of the dehumidifiers represent the industrial state of art. The 3D simulation of the coupled heat and moisture transfer has been performed with Comsol Multiphysics - Heat Transfer Module 4.3b (heat transfer in fluid by forced convection due to dehumidifiers functioning and transport of diluted species to reproduce humidity field). For a realistic prediction of moisture distribution in the storage facility exposed to external climatic conditions, ambient temperature and humidity level are considered in the model (taken from meteorological data). The performance of two different kinds of industrial dehumidifier are compared in order to choose the optimal configuration (layout) to implement within storage facility. The dehumidifiers considered during the simulations differ in terms of handled mass flow and condensation capacity. The scope of this work is to define the kind, the number and the position of industrial dehumidifiers, limiting the existence of stagnated flow regions, thus reducing the drum corrosion risk. An estimate of dehumidifiers' workload, in terms of functioning hours and condensate water production is also provided.

2. Numerical Model

In this section are presented the physical-geometrical features of waste storage, the simplified approach to take into account the ambient temperature variation and the technique used to model the dehumidifier functioning. Are also described the numerical method to model moist air transport and the governing equations.

2.1 Waste Storage: Physical and Geometrical Features

The following Figure 1 and Figure 2 show the plan and a section of the disposal. The external dimension are 35,14x17,74x7,06(h) m and the peripheral concrete wall thickness is 0,5 m. The outer doors are in carbon steel as the waste drums.

The present study regards only the local n. 2 where the drums are shielded by concrete shells.

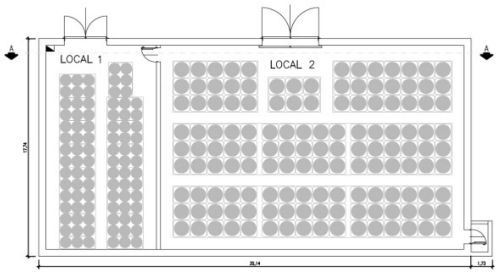

Figure 1 Plan of waste disposal divided in local 1 and local 2.

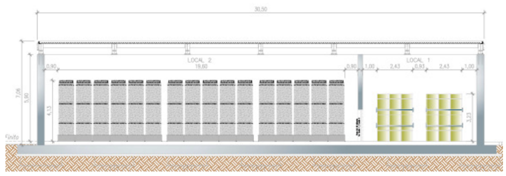

Figure 2 Section A-A of waste disposal.

2.2 Simplified approach for temperature variation

The ambient temperature outside waste disposal T_a is available from meteorological data (annual base). It is also available the irradiation for the specific site (PVGIS web site [2]), therefore the external disposal fictitious wall temperature T_f is known and is defined as [3]:

$$T_f(t) = T_a(t) + \frac{\varepsilon_w I(t)}{h} \qquad (1)$$

where ε_w is the disposal external wall emissivity, h is the radiation-convection heat exchange coefficient and I is the irradiation average on the disposal wall. T_f is a periodic function and can be expressed by Fourier Series:

$$T_f(t) = T_m + \sum_{n=1}^{\infty} (a_n \cos nt + b_n \sin nt) \qquad (2)$$

The theory of transient conduction in a semi-infinite solid subjected to a sinusoidally varying temperature on its exposed face is used to calculate the wall internal face of the disposal T_w (and also for the carbon steel door) [3]:

$$T_w(t) = T_m + \sum_{n=1}^{\infty} b_n e^{-\beta_n s} \sin(\omega\tau_n - \beta_n s) \qquad (3)$$

where the coefficients β_n and τ_n are material dependent, while s is the matter thickness. Substituting in the previous equation the physical and geometrical properties of concrete disposal boundaries the series vanish to zero. Differently from the previous case, for the carbon steel door the fundamental harmonic term (period 24 h) doesn't vanish and must be implemented in the simulation. Considering equation (1) and (2) can be seen that T_m is different for concrete wall and steel door but the difference is less than 2°C. For simplicity will be considered an average value. Due to high thermal inertia the drums surface temperature is considered constant and equal to T_m. The meteorological data used for the external temperature includes also the variation of relative humidity in time.

2.3 Modeling of dehumidifiers functioning

The next figure represents an example of state of art characteristic curves of an industrial isothermal dehumidifier.

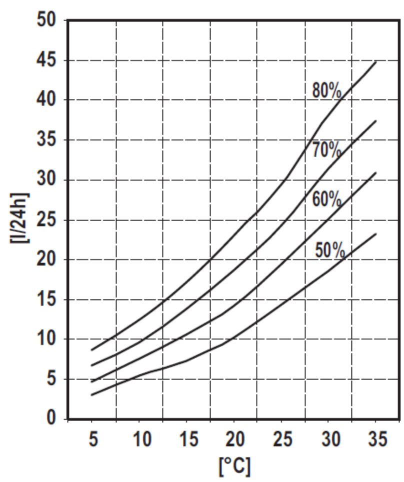

Figure 3 An example of industrial dehumidifier characteristic curves: the condensation capacity, expressed in l/24h, is a function of temperature and relative humidity RH (curve parameter).

The Comsol model imports industrial characteristic curves data of condensed water capacity in time q_c in l/24h as function of air temperature T and relative humidity Φ by interpolation functions tool (interpolation linear and extrapolation constant available for 2D functions).

$$q_c = f(T, \Phi) \quad (4)$$

The simulations are based on the use of two different kind of dehumidifiers. The dehumidifiers kind "A" has a capacity of 33l/24h @ 32°C and RH 90% (air mass handled 380 m^3/h) and the Figure 3 reports its characteristic curves. The dehumidifiers kind "B" has a capacity of 45l/24h @ 32°C and RH 90% (air mass handled 600 m^3/h).

2.4 Moist air transport

The theory used assumes that the moist air is an ideal gas and that the vapor phase concentration field can be described by the equation of transport of diluted species through diffusion and convection terms (see equation 8). The concentration is defined as the ratio between the amount of water vapor in mol and the total volume of mixture considered in m^3. The relative humidity, directly linked to corrosion risk, is defined as the ratio between the water vapor partial pressure and saturation pressure of water vapor (or the ratio of actual concentration and saturation concentration). The saturation state is reached when the relative humidity is one that is when the partial pressure of the water vapor is equal to the saturation pressure (which depends on the temperature too). The transport of diluted species theory assumes that all species present are dilute; that is, that their concentration is small compared to a solvent. As a rule of thumb, a mixture can be considered dilute when the concentration of the solvent is more than 90 mol% (case of study). Due to the dilution, mixture properties such as density and viscosity can be assumed to correspond to those of the solvent.

2.5 Governing equations

The heat and moisture transfer processes in fluid domains can be described by a system of partial differential equations derived by imposing the equilibrium balance of mass (5), momentum (6), thermal energy (7) and concentration of species (8) within an infinitesimal element of volume. The governing equations, for incompressible case are reported in tensor form:

$$\nabla \cdot \boldsymbol{u} = 0 \quad (5)$$

$$\rho \frac{\partial \boldsymbol{u}}{\partial t} + \rho(\boldsymbol{u} \cdot \nabla)\boldsymbol{u} = \nabla \cdot [-p\boldsymbol{I} + \boldsymbol{\tau}] + \boldsymbol{F} \quad (6)$$

$$\rho C_p \left(\frac{\partial T}{\partial t} + (\boldsymbol{u} \cdot \nabla)T\right) = \nabla \cdot (k\nabla T) + \boldsymbol{Q} \quad (7)$$

$$\frac{\partial c}{\partial t} + \boldsymbol{u} \cdot \nabla c = \nabla \cdot (D\nabla c) + R \quad (8)$$

where $\boldsymbol{u}$ is the velocity vector, T the temperature and c the water vapor concentration. For the other terms please refer to Comsol Multiphysics Reference Manual [4].

3. Use of COMSOL Multiphysics

The simulation is performed with Comsol Multiphysics 4.3b – Heat Transfer Module and is based on the following steps: 1) stationary fluid flow study (single-phase incompressible turbulent k-eps closure model); 2) time dependent fully coupled heat and moisture transfer study (heat transfer in fluid by forced convection and transport of diluted species to reproduce humidity field). For the second step, temperature and relative humidity represent the dependent variables, whereas position and time are the independent variables of the problem. The following sections summarize the geometry of computational domain, the mesh and the solver set-up for each simulation step.

3.1 Computational domain and machines layout

The geometrical dimensions of the waste disposal for the three dehumidification machines layout investigated are introduced into COMSOL Multiphysics 4.3b and are shown in Figure 4 and Figure 5. The Layout 1 consist of four dehumidifiers of kind "A" positioned along the walls of the local 2 (Figure 6). The layout 2 is characterized by the use of two dehumidifiers of kind "B" positioned along the left wall of the local 2 (Figure 6). Respect to Layout 2, the Layout 3 differs only for the position of the dehumidifiers, placed at the opposite corners of local 2 (Figure 6). All measures are reproduced in 1:1 scale. The model includes the dehumidifiers chassis, their inlet and outlet sections (for more detail see Figure 4), the door shape and the envelope profile of drums' pile. The interstices between the drums aren't considered for simplicity. This simple geometry is in fact suitable to model the general behavior of the air flows and humidity transport.

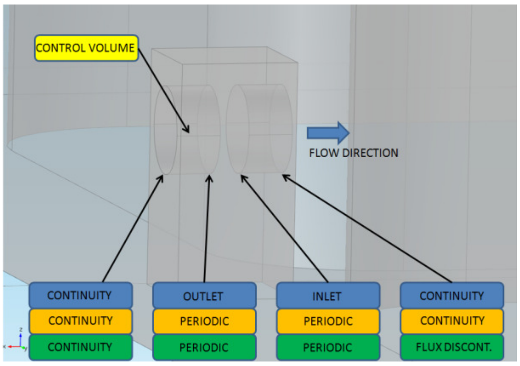

Figure 4 Dehumidifier scheme with the indication of flow direction and boundary conditions applied: in light blue fluid-dynamics, in orange thermal and in green chemical conditions.

3.2 Mesh

In the COMSOL simulations is used an automatic generation of the mesh based on tetrahedral network of 437000 elements with average element quality 0.469 (minimum quality 0.003). A finer mesh is used near the wall and where are expected high gradients. This mesh proved to be dense enough to yield sufficiently accurate results and for a reasonably short simulation time (6 hours for the stationary step and 1 h for non-stationary on a workstation Intel Xeon CPU @2.40 GHZ, 64 GB RAM).

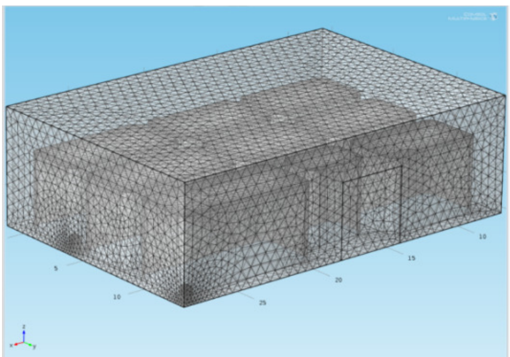

Figure 5 Mesh used for the first layout

3.3 Solver set-up for stationary step

The stationary step is used to obtain the velocity field inside the waste due to dehumidifiers running. The physic selected is single-phase turbulent flow with k-eps formulation as closure model (wall function). As described in § 2.5 the flow is considered incompressible. The following boundary conditions are imposed: atmospheric pressure with no viscous stress option on one dehumidifiers outlet section (velocity conditions for the other outlet surfaces), logarithmic wall function on model's walls (waste disposal wall, dehumidifiers chassis and drum surfaces), velocity inlet condition on all dehumidifiers inlet sections (Figure 4). The inlet and outlet velocity conditions consist of normal velocity imposed on boundary surfaces. The velocity magnitude is expressed by:

$$v = \frac{q_f}{3600 \cdot S} \tag{9}$$

where a q_f is the volumetric flow handled by dehumidifiers in m^3/h (from data sheet) and S is its inlet/outlet surface. The direct, MUMPS, segregated solver configuration is used during the simulation.

3.4 Solver set-up for time dependent step

The time dependent fully coupled heat and moisture transfer step is used to obtain the evolution in time of humidity field into waste disposal, after the door opening (initial condition t=0), during a critical ambient condition day (RH= 85%, T= 32°C). At t=0 is assumed that the moist air concentration and temperature inside the disposal is equal to the external conditions and that the dehumidifiers are working. The time dependent step use the velocity field obtained in the previous study (stationary). The heat transfer in fluid occurs in fact by forced convection and influences the RH field (fully coupled simulation). The physics selected in this step are heat transfer in fluids (turbulent flow) and transport of diluted species (by convection and diffusion). For the first physic the following boundary conditions are applied: constant temperature for concrete walls and drums shells surface ($T_w(t) = T_m$), adiabatic condition on the disposal's floor, on the wall that divides the local 2 from local 1 and on dehumidifiers chassis, periodic heat condition on the inlet and outlet dehumidifiers sections (Figure 4), while for carbon steel door is imposed equation (3) simplified:

$$T_w(t) = T_m + b_{24h} e^{-\beta_{24h} s} \sin(\omega\tau_{24h} - \beta_{24h} s) \tag{10}$$

where a b_{24h} is the amplitude of harmonic term of period 24 h of decomposition in Fourier series (see equations 2 and 3). For the specific case the damping factor $e^{-\beta_{24h}s}$ is close to 0,6 , b_{24h} near to 18°C while the phase shift $\beta_{24h}s$ is 15° (nearly one hour).

For the second physic the moist air diffusion coefficient is assumed equal to $2{,}5\cdot 10^{-5}$ m^2/s and the following boundary conditions are imposed: no flux for all the surfaces except that for inlet, outlet and auxiliary sections of dehumidifiers (Figure 4). Periodic condition is used for the inlet and outlet dehumidifiers surfaces, while for auxiliary section the following flux discontinuity per unit of surface (mol/m^2s) condition is forced (see also (4)):

$$N_{0,c}(T,\Phi) = -\frac{q_c(T,\Phi)}{3600\cdot 24}\cdot\frac{1000}{M_{H2O}\cdot S} \qquad (11)$$

where q_c is the dehumidifiers condensed water capacity in time in l/24h, M_{H2O} is the water molar mass in g and S is the auxiliary section surface. For each dehumidifier the variable T and Φ are the average values in its control volume (calculated each time step through Comsol average operator tool, see Figure 4). The direct, MUMPS, segregated solver configuration is used during the simulation.

4. Results

In this section are presented the results of numerical simulations. The first column of Figure 6 represents the velocity field, the second column the surface relative humidity RH after 7200 s for each layout studied. The first row represent the results for Layout 1, the second for the Layout 2 and the third for the Layout 3. Observing the first column of Figure 6, it can be seen that the Layout 1 reduces the existence of stagnated flow regions even if the maximum velocity is only 2,05 m/s (for the other layout is close to 3,1 m/s). Only the smaller drums pile is affected by a low velocity field around it. The velocity field for the other layout is similar in terms of extension of low velocity areas. The Layout 3, respect to Layout 2, is characterized however by higher velocity around the disposal wall (external short circuit). The second column shows the surface RH field after 7200 s. Due to higher condensed capacity of Layout 1 a low RH global level can be observed during time. Reasonably the difference between Layout 2 and Layout 3 is connected with the short circuit of Layout 3, highlighted before (the condensation capacity of the dehumidifiers increases with humidity level RH and temperature). The drums surface RH peaks have different positions and reach the value 1 on the chassis of the dehumidifiers except for Layout 1. The minimum RH values are localized on the door due to higher temperature respect to the disposal walls.

The first column of Figure 7 represents the volume average and the maximum drums surface RH for the layout investigated. The second column refers to the variation of condensation capacity in time for each dehumidifier. The dehumidification parameters of Layout 2 are similar to Layout 1 despite the reduced number of machines. The Layout 3 is characterized by low dehumidification efficiency and greater difference between the volume average and the maximum drums surface RH. The second column shows the variation of the dehumidifiers efficiency due to their positioning.

5. Conclusion

In this study the capability of COMSOL Multiphysics for solving three-dimensional heat and moisture transfer problems is shown.
The study allowed to choose the optimal machine layout configuration (Layout 2) limiting the existence of stagnated flow regions and, at the same time, increasing machines efficiency, so that the drum corrosion risk is reduced.

6. References

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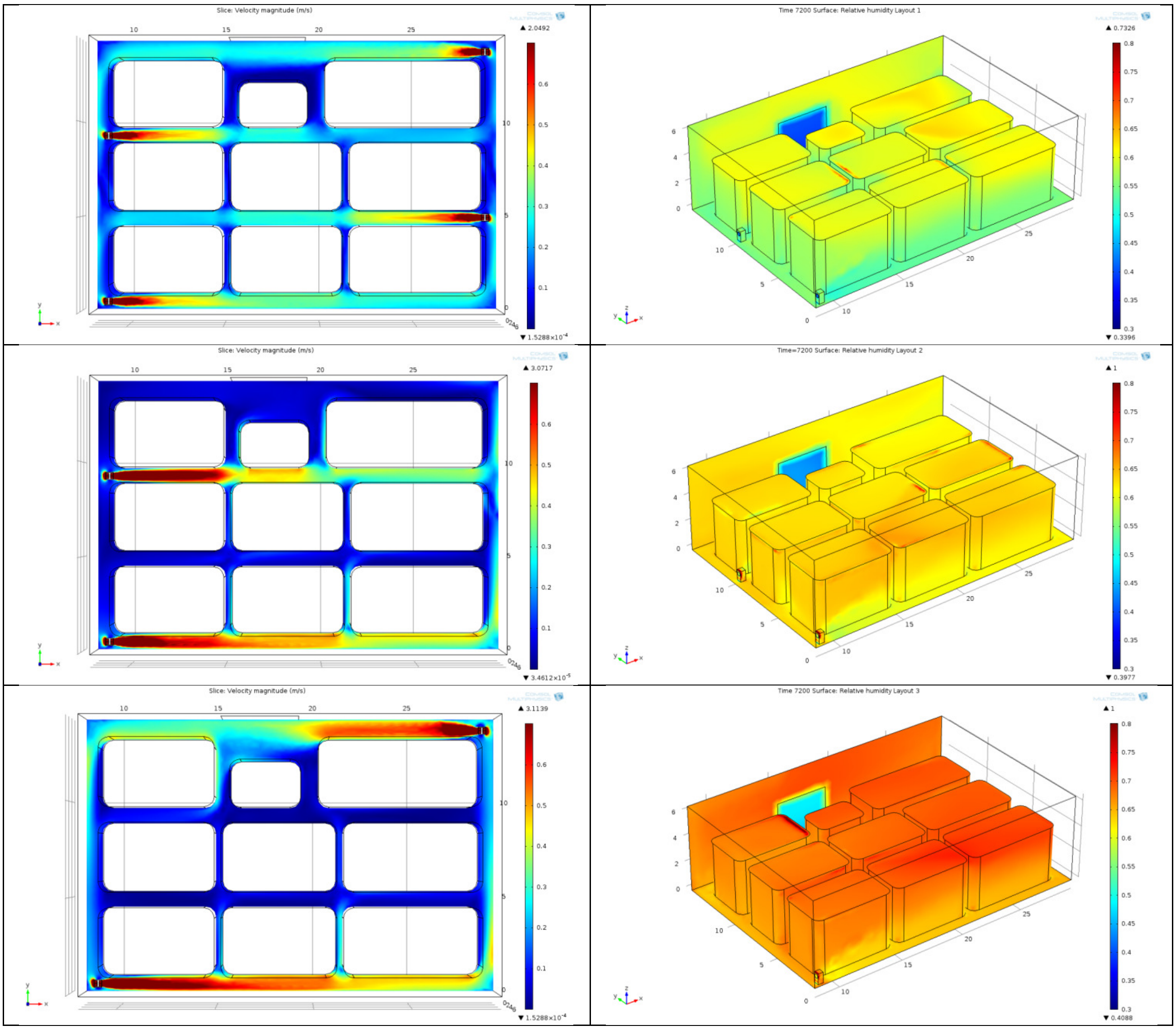

Figure 6 Velocity field and RH surface: the first column represents the velocity field, the second column the surface relative humidity RH after 7200 s for each layout studied. The first row represent the results for Layout 1, the second for the Layout 2 and the third for the Layout 3. For each column the color range is the same.

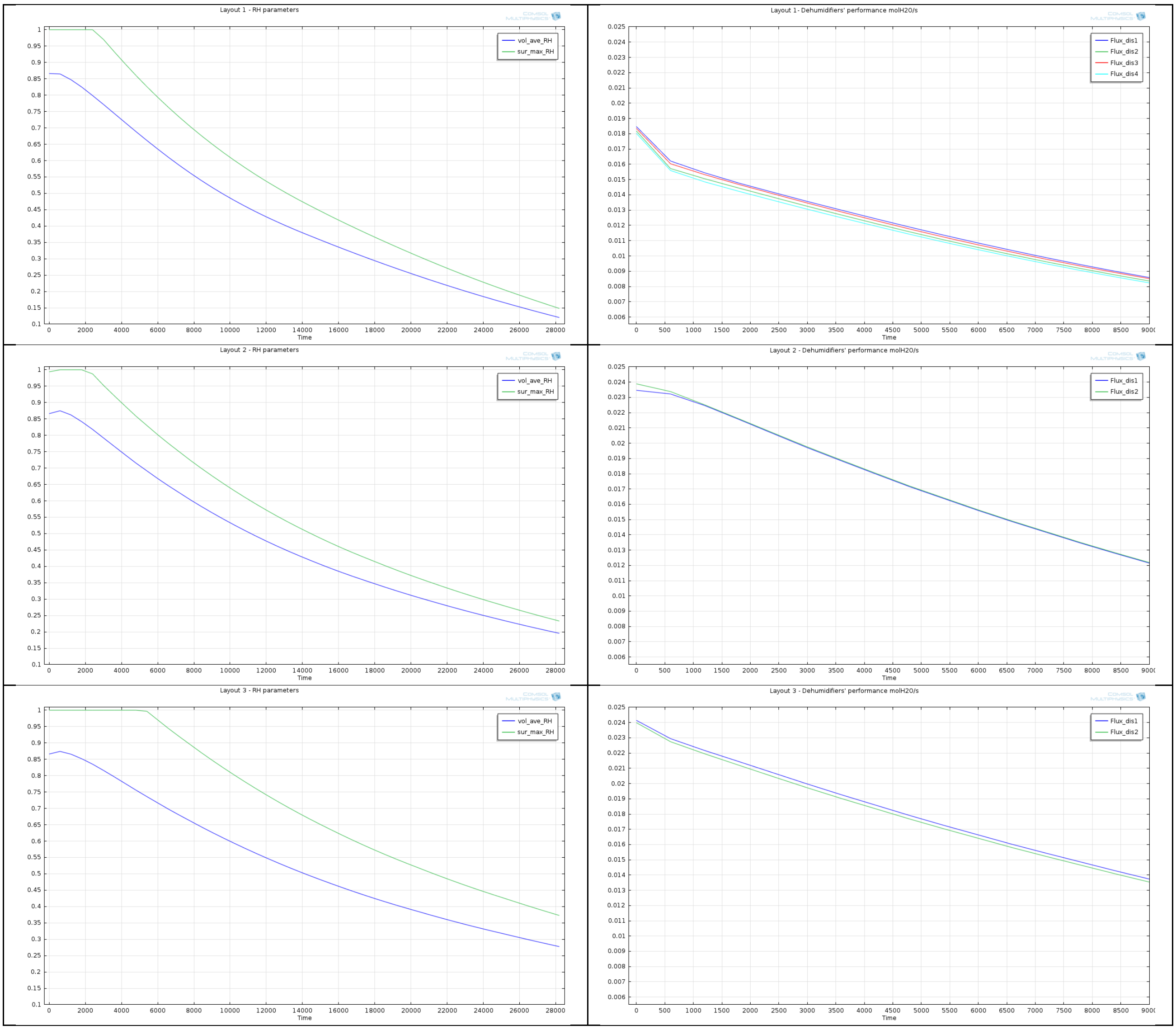

Figure 7 RH parameters and dehumidifiers performance: the first column 7 represents the volume average RH and the maximum drums surface for the layout investigated. The second column refers to the variation of condensation capacity in time (molH2O/s) for each dehumidifier. The dehumidifiers are numbered clockwise from the lower left. For each plot the axis limits are the same.