AN INVERSE PROBLEM METHODOLOGY FOR ESTIMATING HEAT AND DESICCANT WHEELS OFF-DESIGN PARAMETERS

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ABSTRACT

The mathematical modeling of regenerators has been adressed over the years, and has reached a stage of maturity, allowing for the dynamic response of heat and desiccant wheels to be simulated as a function of several non-dimensional design parameters. Although the values of such parameters are set at the design stage, the continuous operation can lead to significant deviation of the original design values. Accordingly, a methodology for retriving the actual operation values of design parameters (such as heat and mass convective coeffcientes) from temperature and measurements is presented. The propsed algorithm carries out a minimization of the difference between calculated and the measured data, which is used as a norm in the search of the parameters. The results show that the proposed methodology estimates the practical values of the parameters with satisfactory accuracy, and can be used as an effective predictive mantainance tool for regenerators and desiccant wheels.

INTRODUCTION

Regenerators can be generally classified as indirect heat exchangers, since the heat transfer between hot and cold stream is mediated by a solid matrix, which is alternatively exposed to each stream. Although there are a number of configurations available, regenerators have in common a great transfer area per unit volume. The reversed flow through the core also allows for an unburdened cleaning schedule, when compared to a parallel plate heat exchanger. Nevertheless, the continuous deposition of particles and oxides eventually contribute to an overall thermal resistance increase. The fouling layer modifies the heat transfer coefficient from the clean start up value, and is progressively detrimental to the effectiveness [1]. Moreover, temperature difference between cold and hot cycles can concur to gasket failure, allowing for air leakage. In the case of rotary regenerators, leakage can occur through the seals which separates the streams, or through the circumferential gap between the rotor and housing [2]. In any case, an off-design mass flow rate will lead to a variation of the regenerator capacity ratio, which also impacts the heat and mass recovery efficiency. Since both fouling and air leakage affect the system performance, it is not possible to credit an effectiveness decrease to one or other (or both) factor, a priori. Accordingly, the present work proposes a parameter estimation methodology for heat and desiccant wheels based on transient temperature outlet measurements. An ill-posed problem is proposed and solved, using the Levenberg-Marquadt algorithm [3,4] to carry out the minimization between measured and calculated temperatures.

NOMENCLATURE

A	[m^2]	Heat transfer area
Bi	[-]	Biot number
C_p	[J/kg K]	Air specific heat at constant pressure
C_r*	[-]	Non-dimensional capacity Ratio
d	[m]	Wall thickness
f	[-]	Desiccant mass fraction
h	[K]	Temperature
H	[J/kg K]	Enthalpy
J	[-]	Sensitivty Matrix
k	[m^2]	Heat transfer conductivity
k_y	[m^2]	Masst transfer conductivity
m	[kg]	Mass
$\dot{m}$	[kg/s]	Mass flowrate
NTU	[-]	Biot number
P	[J/kg K]	Air specific heat at constant pressure
PR	[s]	Periodof revolution
Q	[m]	Wall thickness
R	[-]	Separation factor
t	[s]	Time
T	[K]	Temperature
W	[kg/kg]	Absolute humidity (solid)
x	[m]	Cartesian axis direction
y	[m]	Cartesian axis direction
Y	[kg/kg]	Absolute humidity (air)
Special characters		
λ	[-]	Non-dimensional parameter
θ	[-]	Non-dimensional temperature
μ	[-]	Search weight factor
$\mathcal{\Pi}$	[-]	Half z directional dimension of rectangular cooling
Ω	[-]	Auxilary matrix
Subscripts		
1		Auxiliary index
2		Auxiliary index
3		Auxiliary index
a		Air
*		Non-dimensional
c		Cold period
$calc$		Calculated

h	Hot period
k	Iteration counter
meas	Measured
T	Volumetric effective expression
w	Wall
wc	Wall (cold)
wh	Wall (hot)
y	Mass transfer

The prediction of fouling growth has been addressed by stochastic [5] and mechanistic models [6]. The evaluations of correlated quantities, such as the pressure drop C-factor have been proposed as mechanisms of fouling prediction [7]. As for inverse design, a parameter-estimation technique was able to predict within 10% accuracy the parameters of a specific fouling correlation for crude oil distillation [8]. The conjugate gradient inverse method has been successfully used to predict the fouling layer profiles in pipe internal walls [9]. In addition, experimental techniques such as ultrasonic wave techniques have been developed and applied [10,11], however providing only qualitative indications of fouling.

In addition to the heat recovery, regenerators can also allow for mass recovery, provided the porous matrix is coated with a hygroscopic layer. Desiccant rotors were originally applied in environments which require a thorough humidity control, such as the production of pharmaceuticals and ammunition, grain transport, industrial printing and painting processes [12]. In tropical humidity climates, the use of a desiccant wheel in air-conditioning systems can significantly mitigate the latent load, unburdening the cooling coil [13,14]. Although external air should be properly filtered, the desiccant layer is unavoidably exposed to fine particles, organic compounds and other contaminants which often deposit in the micro-pores, hindering the adsorptive capacity. Moreover, the continuous temperature swing can cause desiccant aging by degradation the crystalline structure. Silica-gel and Alumina have been reported to significantly age for a 200°C regeneration temperature [15]. Microwave regeneration [16] has been suggested as a way of circumventing the thermal fatigue of the desiccant structure. Accordingly, convective heat and mass transfer coefficients and the adsorption heat will be retrieved from humidity and temperature simulated measurements. Parameter estimation techniques have been successfully applied to similar problems, such as the determination of convective coefficients in column adsorption reactors [17], solid-liquid systems [18] and porous slabs [19].

MATHEMATICAL MODELING

The Direct Problem – Heat Wheel

Figure (1) describes the computational field, detached from a transversal section of the regenerator. The model is developed under the simplifying assumptions:

1) The thermal capacitance of hot and cold streams is negligible. When compared to the matrix thermal capacitance.
2) Thermo physical properties are constant.
3) The flow in the channel is hydrodynamically developed
4) The hot and cold flow rates are balanced.
5) Constant fluid and material temperatures in any cross section of the channel (lumped formulation in the y-direction)
6) The regenerator is perfectly insulated.
7) Convective coefficients are uniformly distributed along the flow.
8) Due to the thickness/length ratio, thermal conductance within the storage material is negligible in the flow direction and finite in the normal direction to it.

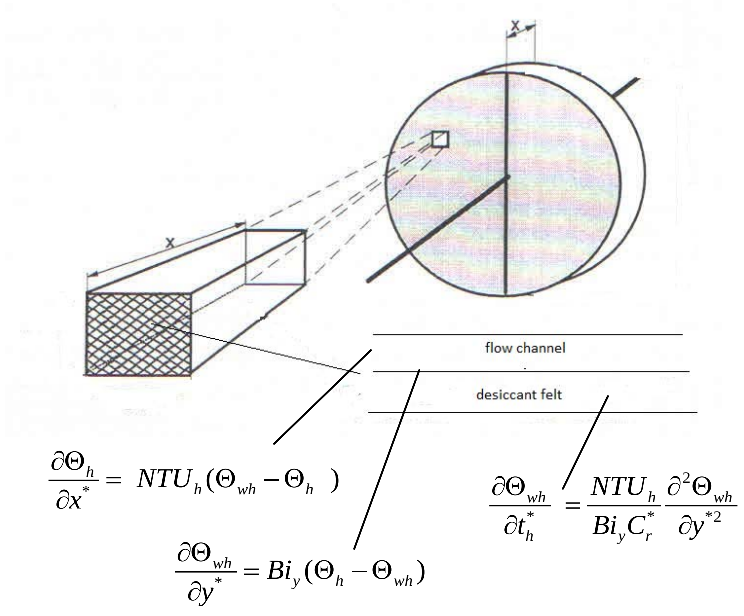

Figure 1 Computational domain (regenerator)

Once energy balances are carried out over elementary control volumes representing the solid matrix and the flow channel, the following set of equations representing the sub sequential exposure to the flow streams (hot and cold periods) is obtained:

$$\frac{\partial \Theta_h}{\partial x^*} = NTU_h(\Theta_{wh} - \Theta_h) \tag{1}$$

$$\frac{\partial \Theta_{wh}}{\partial t_h^*} = \frac{NTU_h}{Bi_y C_r^*}\frac{\partial^2 \Theta_{wh}}{\partial y^{*2}} \tag{2}$$

$$\frac{\partial \Theta_c}{\partial x^*} = NTU_c(\Theta_{wc} - \Theta_c) \tag{3}$$

$$\frac{\partial \Theta_{wc}}{\partial t_c^*} = \frac{NTU_c}{Bi_y C_r^*}\frac{\partial^2 \Theta_{wc}}{\partial y^{*2}} \tag{4}$$

The boundary conditions are given by

$$\frac{\partial \Theta_{wh}}{\partial y^*} = Bi_y(\Theta_h - \Theta_{wh}) \quad at \quad y^* = 1 \tag{5}$$

$$\frac{\partial \Theta_{wh}}{\partial y^*} = 0 \quad em \quad y^* = 0 \tag{6}$$

The non-dimensional parameters are defined as

$$Bi_y = \frac{hd}{k} \tag{7}$$

$$NTU_{h,c} = \frac{hA}{\dot{m}c_p} \tag{8}$$

$$C_r^* = \frac{m_w c_w / PR}{\dot{m}c_p} \tag{9}$$

The domain is discretized into finite-volumes in both directions. Further details on the model and validation are available in the literature [20-22]. In brief, convective terms are represented by an upwind scheme, whereas the transient terms are represented by a fully-implicit scheme, so as to keep the solution stable [23]. The absence of diffusion in the longitudinal direction allows for a line-by-line tri-diagonal matrix algorithm to be applied [24]. In addition, the periodic nature of the problem requires an iterative solution: The initial temperature field along the matrix is arbitrarily set as initial condition. Then calculations are carried out for a complete cycle, and the temperature field at the end of the cycle is compared to the initial guess, replacing it until a convergence criterion is met (less than 0.1% for all calculations). For small values of Bi, the solution evolves to the classical solution for the effectiveness of regenerators [25], which neglects any conductive thermal resistance.

The Direct Problem – Desiccant Wheel

Consider a single flow channel as shown in Figure (2).Some additional assumptions are required:

- Temperature and concentration distributions in the direction normal to the flow are taken to be uniform (lumped) within the channel and the solid.
- The adsorption heat is modeled as a heat source within the flow channel.

Details of the mathematical model development and validation are widely available in the literature. [26-29]. In short, energy and mass balances are applied to elementary control volumes enclosing the sorbent layer and the flow channel, resulting in equations (10) to (13), and an algebraic equation (14) which relates the adsorptive capacity as a function of the vapor pressure in the pore vicinity, known as isotherm. The parameter R is a measure of the strength of adsorption of a particular desiccant material.

$$\frac{\partial Y^*}{\partial x^*} = \lambda_3 \left(Y_w^* - Y^* \right) \tag{10}$$

$$\frac{\partial W}{\partial t^*} = \lambda_2 \left(Y^* - Y_w^* \right) \tag{11}$$

$$\frac{\partial T_a}{\partial x^*} = T_w - T_a \tag{12}$$

$$\frac{\partial T_w}{\partial t^*} = \left(T_a - T_w \right) + \lambda_1 \left(Y^* - Y_w^* \right) \tag{13}$$

$$\frac{W}{W_{\max}} = \frac{1}{(1 - R + \frac{R}{\phi_w})} \tag{14}$$

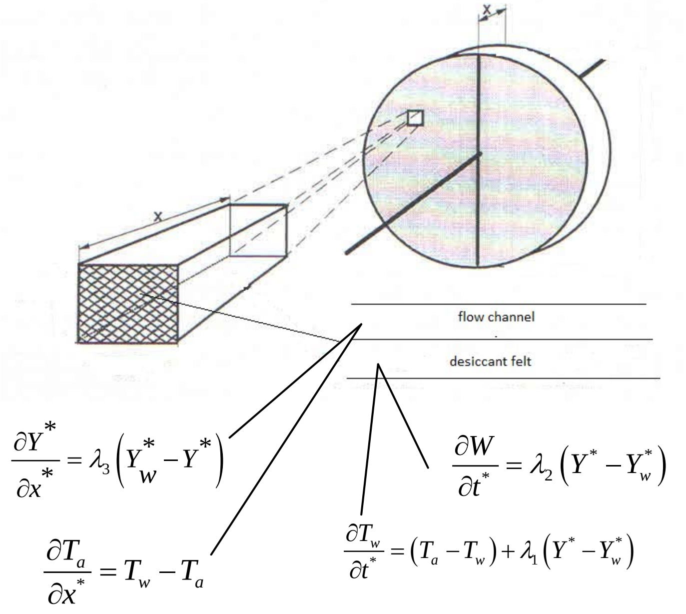

Figure 2 Computational domain (desiccant wheel)

$$\lambda_1 = \frac{Q}{\left(\frac{\partial H_a}{\partial T_a} \right)} \tag{15}$$

$$\lambda_2 = \frac{C_{wr}}{f \left(\frac{\partial H_a}{\partial T_a} \right)} \tag{16}$$

$$\lambda_3 = \frac{k_y}{h} \left(\frac{\partial H_a}{\partial T_a} \right) \tag{17}$$

Overall heat and mass balances are applied as acceptance criteria of the obtained solutions. Both R and λ_1 represent properties of the desiccant material, which are unlikely to be affected by fouling. Conversely, the continuous deposition of particles can lead to micro-pores obstruction and extra thermal resistance, thereby affecting the values of λ_2 and λ_3.

The Inverse Problem

Parameter and function estimation techniques have been applied to a wide range of heat transfer problems. In particular, the retrieval of parameters P_1 and P_2 (which represent NTU and Cr* for the heat wheel and λ_2 and λ_3 for the desiccant wheel) from temperature measurements will follow the Levenberg-Marquadt algorithm. To validate the methodology, a simulated experiment will be carried out. The direct problem is solved with prescribed (real) values for parameters P_1 and P_2. Then, 40 air outlet temperature values (at equally spaced time intervals) are recorded and a perturbation by a random parameter (with Gaussian distribution) with a given standard deviation is applied, so as to simulate an array of temperature measurements. This "measured" temperature vector is the used to feed the algorithm, which is expected to retrieve the original parameters which generated the temperature vector. The objective function (norm) is given by the difference between measured and calculated temperatures, which is to be minimum when the latter is evaluated using the correct estimated values for the parameters, which comprise the parameter vector **P**. In short, the estimative of the parameter vector **P** involves the following procedure:

1. Solve the direct problem with initially guessed values for the vector $\mathbf{P}^k$ and obtain a solution vector $\Theta_{wh,\pi}\left(\mathbf{P}^k\right)$, which represents the (calculated) temperature values. Then add a perturbation to each vector element by a random value with specified maximum magnitude $\delta\mathbf{\Theta}$, so as to obtain a "measured temperatures" with known accuracy.

2. Calculate the norm according to

$$S\left(\mathbf{P}^k\right)=\left[\Theta_{calc}-\Theta_{meas}\left(\mathbf{P}^k\right)\right]^T\left[\Theta_{calc}-\Theta_{meas}\left(\mathbf{P}^k\right)\right] \tag{18}$$

3. Calculate the sensitivity matrix according to

$$\mathbf{J}\left(\mathbf{P}\right)=\left[\frac{\partial\Theta^T\left(\mathbf{P}\right)}{\partial\mathbf{P}}\right] \tag{19}$$

4. Calculate the auxiliary matrix Ω_k according to

$$\mathbf{\Omega}^k = diag\left[\left(\mathbf{J}^k\right)^T\mathbf{J}^k\right] \tag{20}$$

5. Solve the following algebraic system for the search step vector

$$\Delta\mathbf{P}^k=\left[\left(\mathbf{J}^k\right)^T\mathbf{J}^k+\mu^k\Omega^k\right]^{-1}\left(\mathbf{J}^k\right)^T\left[\Theta_{meas,wh,\pi}-\Theta_{wh,\pi}\left(\mathbf{P}^k\right)\right] \tag{21}$$

6. Calculate the new estimative vector, solve the direct problem with the new estimative $\mathbf{P}^{k+1}$ and calculate the next norm. The next norm is compared to the current one, replacing it whenever lower. In that case, accept the new estimative and proceed to step 8. Replace μ^k by $10\mu^k$ and return to step 5, otherwise.

7. Replace μ^k by 0.1 μ^k, and check for convergence. Return to step 3 while convergence has not been attended. Cease the calculations otherwise.

Results

The analysis of the sensibility coefficients is of the prime importance in inverse problems. For the heat wheel problem, Figure (3) shows the square of the sensitivity coefficients along the hot period. The periodic nature of the problem has a strong influence over J_1 (associated to C^*_r), which exhibits a peak at half of the period. Conversely, the sensitivity coefficient associated to NTU (J_2) is continuously decreasing, as the fluid and the channel wall progress to thermal equilibrium by the end of the period. Also, the comparison of the curves shows the sensitivity coefficients are uncorrelated, allowing for the simultaneous estimation of NTU and C_r*, and the problem sensitivity to the later is greater than that of the former. Table (1) shows calculated parameters for two case studies, as a function of the maximum deviation from the exact solution. The results were obtained for a variety of initially guessed values, indicating good convergence and stableness of the method. The calculated parameters show excellent agreement with the real values, once the norm meets pre-established convergence criteria. The worst prediction was found to have a 6.2% discrepancy over the correct value, for a non-dimensional temperature perturbation of 0.01. This would correspond to a rather coarse measurement error (+-5°C) for high temperature applications. However, for a low temperature application (such as in HVAC projects) this maximum perturbation would correspond to a dimensional error as small as +-0.5°C. Accordingly, the application of the presented methodology to the latter case requires a greater effort in obtaining trustable temperature measurements than that of the former. Table (2) shows the results for the desiccant wheel parameter estimation for two sets of λ_2 and λ_3 values, for random maximum deviations of +-0.5°C and +-1.0°C added to the correct values. It can be seen that very good estimates are obtained in both instances. Figure (4) shows the sensibility coefficients are uncorrelated, which allows for the simultaneous estimation of λ_2 and λ_3, although the sensibility coefficient associated with the former is much higher than that of the later. The continuous growth of J_1 can be explained by considering the definition of λ_2, as given by eq. (16). Consider a positive perturbation of λ_2 as a result of decrease in the desiccant mass fraction f (i.e., a decrease in the amount of desiccant). Physically, this might as well represent micro-pore blockage by fouling, hindering the mass transport. Accordingly, all activation energy is converted into sensible energy, resulting in material overheating and deliquescence. Figure (5) shows the topology of the desiccant wheel problem, in the vicinity of the exact solution.

Table 1 Heat wheel retrieved parameters, cases (a) and (b)

$\delta\Theta$	Tol	Cr*	NTU	Tol	Cr*	NTU
10^{-4}	10^{-7}	2.95	11.96	10^{-7}	4.97	19.99
10^{-3}	10^{-5}	2.97	11.93	10^{-6}	5.15	19.89
10^{-2}	10^{-4}	2.88	11.96	10^{-4}	5.26	19.78
Correct Value		**3.00**	**12.00**		**5.00**	**20.0**

Table 2 Desiccant wheel retrieved parameters

δ**T** (°C)	Tol	λ_2	λ_3	Tol	λ_2	λ_3
0.5	1.0	7.17	0.75	1.0	9.31	0.52
1.0	3.0	7.28	0.74	3.0	9.33	0.54
Correct Value		**7.20**	**0.76**		**9.30**	**0.52**

CONCLUSION

The continuous operation of regenerative exchangers can lead to significant deviation from original design values, which might occur as a consequence of fouling or air leakage. Accordingly, a methodology for the assessment actual parameters of heat and desiccant wheels from temperature measurements along the cycle was developed and validated through a simulated experiment. It was found that the Levenberg-Marquadt algorithm is able to retrieve the actual values for the unknown parameters with great accuracy and a small computational effort, from simple outlet temperature measurements. The proposed methodology can be coupled with monitoring systems so as to provide utility engineers with operation parameters estimates, allowing for the updating of preventive maintenance schedules.

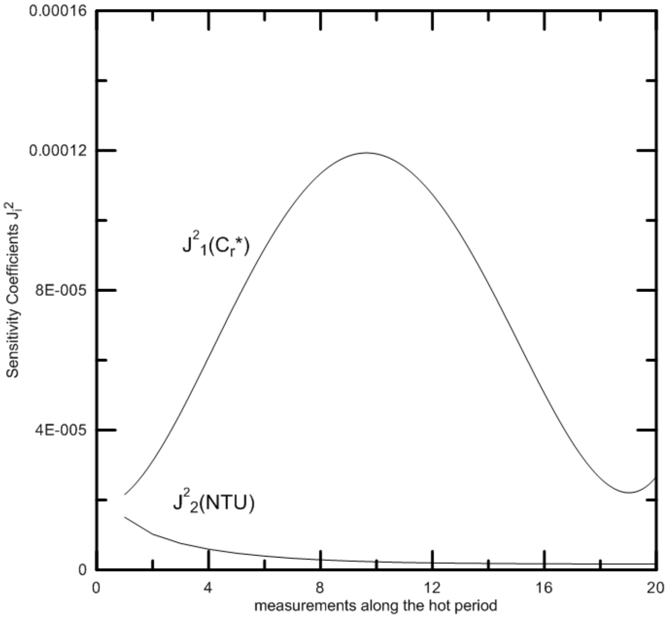

Figure 3 Sensitivity Coefficients for the heat wheel problem

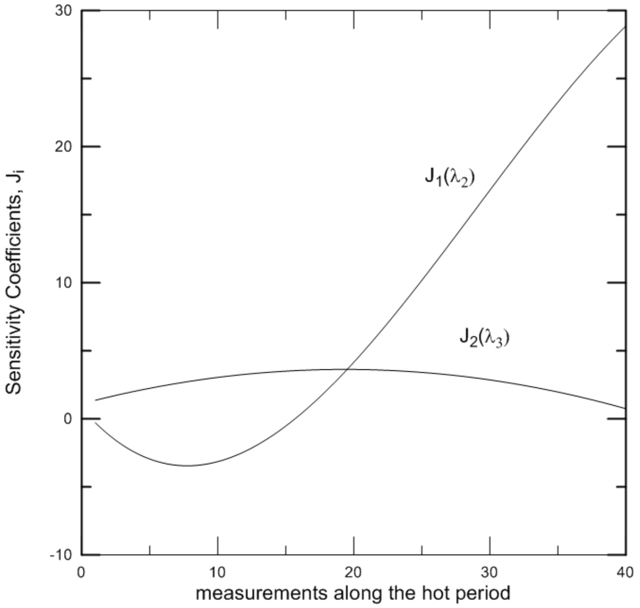

Figure 4 Sensitivity Coefficients for the desiccant wheel

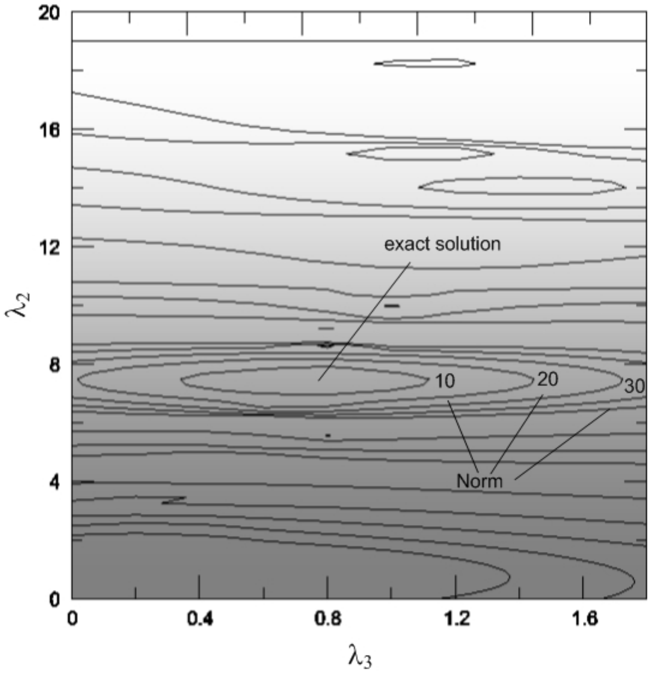

Figure 5 Topology of the Desiccant Wheel Problem

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