Supplementary material

Mateo Arcila-Osorio, Hernán Alvarez and Carlos Ocampo-Martinez

1. Model basic structure

This section presents the derivation of the equations comprising the basic structure of the model, which were presented in Sect. 2 in the chapter. For the convenience of the reader, those equations are displayed here in blue. Besides, in this supplementary material, the nomenclature of the variables, parameters, and constants remains consistent with that used in the chapter.

Conservation principle application

In this step of the Phenomenological Based Semi-physical Modelling (PBSM) approach, material and energy balances are deduced for each of the Process Systems (PSs) previously defined (see Sect. 2 in the chapter).

A. PS_I to PS_{IV} - humid air into conduction and fittings: These PSs share the same behaviour, being only different by the material of the conduction and the type of fittings used for each tubing assembly. There, only momentum exchange takes place without important mass or heat interactions due to the low effect of pressure on total humidity.

- *Total Mass Balances (TMB)*. These four PSs satisfy the continuity of mass at each PS volume. In addition, no concentration changes take place. Therefore, the following trivial total mass balance yields the single equation to apply, without requiring a component mass balance in these four PSs:

$$\dot{m}_{i+1} = \dot{m}_i, \tag{1}$$

Eq. (1) assumes the output stream of each tubing section as unknown. In the following, the thermal energy and mechanical energy balances are discussed. These balances are considered in separate way due to their big difference in magnitude.

- *Thermal Energy Balances (ThEB)*. Isothermal operation is achieved because of the minimal temperature variation between the input and output at each PS, which conducts to constant enthalpy operation $\widehat{H}_{i+1} = \widehat{H}_i$. Therefore, these balances do not give useful information to the model in PS_I to PS_{IV}.

- *Mechanical Energy Balance (MEB)*. This balance is the same for PSs from PS_I to PS_{IV}, indicating with indices i and $i+1$ the inlet and outlet ports of the PS, respectively. The values for i and $i+1$ correspond to the stream circled numbers in the block diagram of the proposed PSs (see Sect. 2 in the chapter). A *MEB* equation or Bernoulli's equation is valid for a gas flowing by a tube if the pressure losses are less than 10% of gas absolute pressure at the tube inlet port [1]. This condition is totally fulfilled in the current process, allowing to use the following *MEB* for this PS:

$$\frac{P_i}{\rho_{a,i}} + g\, z_i + \alpha_i\, \frac{v_i^2}{2} = \frac{P_{i+1}}{\rho_{a_{i+1}}} + g\, z_{i+1} + \alpha_{i+1}\, \frac{v_{i+1}^2}{2} + h_{f_{i\to i+1}}, \tag{2}$$

being P_i the pressure of the stream, $\rho_{a,i}$ the density of the dry air and water vapour mixture, g the gravity acceleration constant, z_i the height or current point with respect to a reference point, α_i the flow regime correction factor, and v_i the velocity, all for the gas mixture at point i. Moreover, $h_{f_{i\to i+1}}$ represents the friction losses due to mixture flow between points i and $i+1$. The factor α_i is a constant indicating either laminar or turbulent flow profile, evaluated in accordance with the Reynolds dimensionless number, i.e., $\alpha = 2.0$ for laminar flow and $\alpha = 1.01$ for turbulent flow.
Considering the mixture density as a constant at each analysed section, and keeping in mind that the tube diameter is also constant for each section, the velocity will be constant too, and both velocity terms can be cancelled from the *MEB*. It should be noted that density changes with pressure losses through long distances, but in this case, the gas density is taken as a constant at each section. Under these assumed conditions, the next final *MEB* equation, without knowing the pressure in the terminal point $i+1$, is obtained as follows:

$$P_{i+1} = P_i - \rho_{a_i}\; g\; (z_i - z_{i+1}) - \rho_{a_i}\; h_{f_{i\to i+1}}, \tag{3}$$

since $\rho_{a_{i+1}}$ is a function of P_{i+1}, determining the value of P_{i+1} would require an iterative process in the calculation program. However, such iterations could significantly escalate computational costs and prolong the overall calculation time. Therefore, to derive Eq. (3) it was additionally assumed that $\rho_{a_{i+1}} = \rho_{a_i}$. This assumption is justified, as the density change due to pressure drop after each PS has a small value (usually less than 10%). Moreover, employing this approach for pressure calculation yields a satisfactory alignment with the data reported in [2], which was utilized for model validation.

B. PS_V – humid air contained into the humidifier: This PS considers all the dry air and water vapour mixture contained into the humidifier, flowing through the Nafion tubes during its humidification by mass transfer effect.

- *Total Mass Balance (TMB)*. The total mass balance for this PS is:

$$\frac{dM_{PS_V}}{dt} = \dot{m}_4 - \dot{m}_5 + \dot{m}_8, \tag{4}$$

Eq. (4) is used as differential equation to evaluate M_{PS_V} or used as algebraic equation to evaluate its change taken as a parameter $\dot{M}_{PS_V} = \dot{m}_4 - \dot{m}_5 + \dot{m}_8$. The values of M_{PS_V} and $\dot{M}_{PS_V}$ are required in subsequent model equations.

- *Component Mass Balances (CMB)*: water vapour. After applied the conservation principle over the water vapour component, the following expression is obtained:

$$\frac{dM_{wv,PS_V}}{dt} = w_{wv,4}\,\dot{m}_4 - w_{wv,5}\,\dot{m}_5 + w_{wv,8}\,\dot{m}_8. \tag{5}$$

Using the equivalence $M_{wv,PS_V} = w_{wv,PS_V}\,M_{PS_V}$ it is possible to apply the derivative, considering $\dot{M}_{PS_V}$ as a parameter. Keeping in mind that the mass fraction of vapour in stream 8 is 1.0 (all this stream is water), and considering that PS_V is perfectly stirred regarding its output stream, the vapour mass fraction of the stream $w_{wv,5}$ is equal to the mass fraction of PS_V as a whole. In this way, the final expression for the vapour component balance is

$$\frac{dw_{wv,5}}{dt} = \frac{1}{M_{PS_V}}\left[w_{wv,4}\,\dot{m}_4 - w_{wv,5}\,\dot{m}_5 + \dot{m}_8 - w_{wv,5}\,\Delta M_{PS_V}\right]. \tag{6}$$

- *Component Mass Balances (CMB)*: dry air. This balance is not required because the mixture is binary, then knowing one of the mass fractions (w_{wv} for water vapour), the other (w_{da} for dry air), is straightforwardly found by using the constitutive equation $w_{da} = 1 - w_{wv}$.
- *Thermal Energy Balance (ThEB)*. The thermal energy balance is expressed as the product of the specific heat capacity of the gas mixture at constant volume $\widehat{C}_{V_a}$, the total mass M_{PS_V}, and the PS temperature T_{PS_V}:

$$\frac{dE_{PS_V}}{dt} = \frac{d(\widehat{C}_{V_{a,5}}\,M_{PS_V}T_{PS_V})}{dt} = -\dot{m}_8\,\widehat{C}_{P_{wv,8}}\,(T_5 - T_8) + \dot{Q}_{T-A}. \tag{7}$$

Then, the derivative is computed under constant heat capacity, keeping in mind that the total mass was previously obtained in Eq. (4). In addition, assuming a perfect stirred system $T_{PS_V} = T_5$. Thus, solving for the derivative of the temperature with respect to time, the final *ThEB* for PS_V is as follows:

$$\frac{dT_5}{dt} = \frac{1}{\widehat{C}_{V_{a,5}}\ M_{PS_V}}\Big[-\dot{m}_8\ \widehat{C}_{P_{wv,8}}\ (T_5 - T_8) + \dot{Q}_{T-A}\Big]. \tag{8}$$

The flow of mechanical work leaving the fluid during its pass through PS_V is evaluated as the frictional losses between the inlet and outlet ports of the section, obtained as a term of the mechanical energy balance. Transforming this mechanical energy into its equivalent thermal energy, a small value of such an energy is obtained. Therefore, as usual in the related literature [3, 4], this energy is neglected in the *ThEB*.

- *Mechanical Energy Balance (MEB)*. The same mechanical energy balance or Bernoulli's equation (Eq. (2)) applied to PSs from PS_I to PS_{IV} is valid here and it is used between points 4 and 5 in Figures in the chapter (see Sect. 2). In this expression, the velocity at the input point is not the same as the velocity at the output point due to the density change of the gas mixture ($\rho_{a,4} \neq \rho_{a,5}$). This density change is due to the mixture heating and water vapour addition given by mass transfer. However, due to the complexity of calculating this density change and to avoid iterations in the computational model, this effect is included and adjusted with the other pressure losses term. The final equation to evaluate the pressure at the humidifier outlet is:

$$P_5 = P_4 - \Delta P_{4\to 5}, \tag{9}$$

grouping all terms of flow and energy losses into the pressure losses term $\Delta P_{4\to 5}$ of humid air flowing through the humidifier tubes. The amount of these pressure losses is given by the humidifier manufacturer at nominal flow. Considering a linear pressure losses variation regarding air flow, a constitutive equation for evaluating those pressure losses will be given in the model extended structure.

C. PS_{VI} – water into the humidifier:

- *Total Mass Balance (TMB)*. For this mass balance, the total mass into PS_{VI} is the product of volume and density of water, considering constant density in this PS since the fluid is liquid water and the temperature change is narrow during the process operation. In addition, the humidifier shield is a vertical cylinder with constant cross area A_{Sh}, and the liquid water volume can be expressed as the product of the effective tank cross area and the liquid level, i.e., $V_{PS_{VI}} = A^*_{Sh}\, L$. The effective tank cross area (A^*_{Sh}) is the total tank cross area minus the area occupied by the Nafion tubes. Using the level $L_{PS_{VI}}$ as the main variable, computing its derivative and replacing it into the typical balance expression, the balance equation is:

$$\frac{dL_{PS_{VI}}}{dt} = \frac{1}{A^*_{Sh}\,\rho_W}\left[\dot{m}_7 - \dot{m}_8\right], \tag{10}$$

being ρ_W the density of liquid water and $\dot{m}_7$ the make-up water to be supplied to the humidifier. Using Eq. (10), it is possible to follow the changes of water level into the humidifier. However, this level is suitably controlled in the current assembly. Therefore, this condition conduces to $\frac{dL_{PS_{VI}}}{dt} = 0$, and then Eq. (10) is reduced to:

$$\dot{m}_7 = \dot{m}_8, \tag{11}$$

a trivial expression to find the make-up water. Nevertheless, it is also a model basic equation.

- *Component Mass Balances (CMB)*. In this PS, the concentration is constant because the fluid is pure water along the process. Therefore, no component mass balances are required.
- *Thermal Energy Balance (ThEB)*. This balance is obtained as for previous PSs, but here with the heat capacity at constant pressure because the water is in liquid phase ($\widehat{C}_{P_{wL}}$). In addition, $T_{PS_{VI}} = T_8$, assuming a perfectly stirred system and null mass change due to the level controller operation. Therefore, the *ThEB* for PS_{VI} is:

$$\frac{dT_8}{dt} = \frac{1}{\widehat{C}_{P_{wL}}\ M_{PS_{VI}}}\Big[-\dot{m}_8\ \lambda_{Vap} - \dot{m}_8\ \widehat{C}_{P_{wL}}\ (T_8 - T_7) + \dot{Q}_{H1-W} - \dot{Q}_{T-A} - \dot{Q}_{Lost}\Big]. \tag{12}$$

- *Mechanical Energy Balance (MEB)*. For this PS, the *MEB* gives trivial information, i.e., the friction losses because of the water movement into the humidifier. Water is supplied due to an On-Off controller during a few seconds when the level is below its set-point. The quantity of supplied water is small since it only corresponds to the water transferred to the air by mass transfer. Hence, pressure losses will be quite small due to the low velocity of water ascending into the cylinder. Mentioned pressure losses have no interest to answer the model question. Thus, a *MEB* for PS_{VI} is not required in this model.

D. PS_{VII} – humidified air:

- *Total Mass Balance (TMB)*. By continuity of mass flow, this balance is trivial. In addition, considering density and the process system volume as constants, the mass remains constant too $\left(\frac{dM_{PS_{VII}}}{dt} = 0\right)$, producing the algebraic equation:

$$\dot{m}_6 = \dot{m}_5, \tag{13}$$

which only confirms the mass flow continuity. However, it is also a model basic equation.

- *Component Mass Balances (CMB)*. In this PS, the mass flow behaviour is similar to that of the mixture in PSs from PS_I to PS_{IV}. Therefore, no *CMB* are required since no changes in gas mixture composition occur.
- *Thermal Energy Balance (ThEB)*. Proceeding in the same way that applied for the other PSs and using the equivalence give by Eq. (13), the *ThEB* here is written as follows:

$$\frac{dT_6}{dt} = \frac{1}{\widehat{C}_{V_{a,6}}\ M_{PS_{VII}}}\Big[\dot{m}_6\ \widehat{C}_{P_{a,6}}\ (T_5 - T_6) + \dot{Q}_{H2-W}\Big]. \tag{14}$$

- *Mechanical Energy Balance (MEB)*. The same *MEB* applied to PSs from PS_I to PS_{IV} is valid here. Despite the possibility of considering that both input and output velocities differ due to density changes in the mixture caused by added heat, this difference is very small. Therefore, no velocity effects are included and density difference is not considered. In addition, the inlet and outlet of this section are at the same height and hydrostatic head effect in gases is negligible. Assuming a turbulent flow ($\alpha_5 = \alpha_6 = 1.0$), the balance equation is:

$$P_6 = P_5 - \rho_{a,5}\ h_{f_{5\to 6}}. \tag{15}$$

Finally, the basic structure is composed of the essential dynamic equations of the model written in blue and reported in Table 1. It should be highlighted that some of these equations produce several expressions since they are written for index i, indicating a section of tube and fittings assembly.

Table 1 Equations of the model basic structure.

Process system	Equations[a]
PS_I to PS_{IV}	$\dot{m}_{i+1} = \dot{m}_i$ $P_{i+1} = P_i - \rho_{a_i}\ g\ (z_i - z_{i+1}) - \rho_{a_i}\ h_{f_{i\to i+1}}$
PS_V	$\frac{dM_{PS_V}}{dt} = \dot{m}_4 - \dot{m}_5 + \dot{m}_8$ $\frac{dw_{wv,5}}{dt} = \frac{1}{M_{PS_V}}\left[w_{wv,4}\,\dot{m}_4 - w_{wv,5}\,\dot{m}_5 + \dot{m}_8 - w_{wv,5}\,\dot{M}_{PS_V}\right]$ $\frac{dT_5}{dt} = \frac{1}{\widehat{C}_{V_{a,5}}\ M_{PS_V}}\left[-\dot{m}_8\ \widehat{C}_{P_{wv,8}}\ (T_5 - T_8) + \dot{Q}_{T-A}\right]$ $P_5 = P_4 - \Delta P_{4\to 5}$
PS_{VI}	$\dot{m}_7 = \dot{m}_8$ $\frac{dT_8}{dt} = \frac{1}{\widehat{C}_{P_{wL}}\ M_{PS_{VI}}}\Big[-\dot{m}_8\ \lambda_{Vap} - \dot{m}_8\ \widehat{C}_{P_{wL}}\ (T_8 - T_7) + \dot{Q}_{H1-W}$ $- \dot{Q}_{T-A} - \dot{Q}_{Lost}\Big]$
PS_{VII}	$\dot{m}_6 = \dot{m}_5$ $\frac{dT_6}{dt} = \frac{1}{\widehat{C}_{V_{a,6}}\ M_{PS_{VII}}}\left[\dot{m}_6\ \widehat{C}_{P_{a,6}}\ (T_5 - T_6) + \dot{Q}_{H2-A}\right]$ $P_6 = P_5 - \rho_{a,5}\ h_{f_{5\to 6}}$

[a] Subindex i denotes the different circled points indicated in Figures provided in the chapter.

2. Model extended structure

This section presents the equations that constitute the extended structure of the model. These equations complement the basic structure, derived in previous section, to construct the complete model. Here, two additional steps of the PBSM approach are applied: the variables, parameters, and constants recognition, and the constitutive and assessment equations determination.

Variables, parameters and constants

Diverse interpretations exist in the literature related to the concept of *variable*. To avoid confusions, the difference among the terms *variable* and *unknown* is here properly established. Variables are always part of the model unknowns, but not all unknowns are model variables. The difference is that variables are determined only after solving the mathematical model. On the other hand, parameters are unknowns for the mathematical set of equations forming the model extended structure, including those parameters fixed by the modeller. All parameters should be identified before any solution of the mathematical model. Constants are known fixed values, which are not susceptible to change. Finally, variables and structural parameters, and the values of the model constants are listed in Tables 2 and 3, respectively.

Table 2 Model variables and structural parameters.

	PS_{ItoIV}	PS_V	PS_{VI}	PS_{VII}	Total
Variables[a]	$\dot{m}_{i+1}$, P_{i+1}	M_{PS_V}, w_{wv_5}, T_5, P_5	$\dot{m}_7$, T_8	$\dot{m}_6$, T_6, P_6	17
Structural Parameters[a]	$\dot{m}_0$, $\rho_{a,i}$, P_0, $h_{f_{i\to i+1}}$	$\dot{m}_5$, $\dot{m}_8$, $w_{wv,4}$, $\dot{M}_{PS_V}$, $\widehat{C}_{V_{a,5}}$, $\widehat{C}_{P_{wv,8}}$, $\dot{Q}_{T-A}$, $\rho_{a,5}$, $\Delta P_{4\to 5}$,	$\widehat{C}_{P_{wL}}$, $M_{PS_{VI}}$, $\dot{Q}_{H1-W}$, $\dot{Q}_{Lost}$	$\widehat{C}_{V_{a,6}}$, $M_{PS_{VII}}$, $\widehat{C}_{P_{a,6}}$, $\dot{Q}_{H2-A}$, $\rho_{a,5}$, $h_{f_{5\to 6}}$	33

[a] Subindex i denotes the different circled points indicated on Figures in the chapter. Note that inlet mass flows and input pressures from PS_I to PS_{IV} only produce two parameters. All other mass flows and pressures are variables given by the model after its mathematical solution.

Constitutive and assessment equations for model parameters

The purpose of this section is to find either constitutive or assessment equations for calculating the largest number of structural and functional parameters for each PS. Those parameters without a constitutive/assessment equation must be either identified from experimental data [5] or determined from a correlation sub-model.

Table 3 Values of model structural and functional constants [6].

Symbol	Description	Value	Units
R	Universal constant for ideal gas	8.31441	$\frac{\mathrm{kPa\,m^3}}{\mathrm{kmol\ \ K}}$
$\mathfrak{M}_{da}$	Molecular mass of dry air	29	$\frac{\mathrm{kg}}{\mathrm{kmol}}$
$\mathfrak{m}_{wv}$	Molecular mass of water	18	$\frac{\mathrm{kg}}{\mathrm{kmol}}$
λ_{Vap}	Water heat of vaporisation	2360	$\frac{\mathrm{kJ}}{\mathrm{kg}}$

The remainder structural parameters have a trivial assessment equation due to they are directly taken from data related to the process operation, i.e., $\dot{m}_0 = \mathtt{Datum}$, $P_0 = \mathtt{Datum}$. It is important to highlight that data are not the same as constant values, because the former can change during operation, being their variations defined by the modeller.
A constitutive equation for a given parameter can produce new parameters, which must be also determined. When a function is used for determining a parameter, new parameters produced by such a function are called functional parameters. The new function is part of the model extended structure and the new parameters should be immediately specified to illustrate the solution sequence of the primitive parameters. In the sequel, a brief rationale about the determination of constitutive and assessment equations for two of the structural model parameters, namely the flow of water vapour due to mass transfer into the humidifier Nafion tubes and the friction energy losses, is presented. Their no-so-short deduction illustrates the procedure followed to find expressions and/or values for all the remainder model parameters.

A. Mass transfer $\dot{m}_8$: for evaluating this mass transfer flow, the following expression is used:

$$\dot{m}_8 = A_M\, M'_{wv}, \tag{16}$$

where A_M is the mass transfer area and M'_{wv} is the flux of mass transfer, both functional parameters, evaluated as follows.
The mass transfer area is calculated from the Nafion tube dimensions and the number of tubes into the humidifier as:

$$A_M = N_{NT}\,(\pi\, D_{Mean,Tube}\, L_{Efec,Tube}), \tag{17}$$

being N_{NT} the number of Nafion tubes, $D_{Mean,Tube}$ the mean diameter of a Nafion tube, and $L_{Efec,Tube}$ the effective height in contact with water liquid of the Nafion tubes. The first new functional parameter is evaluated as $N_{NT} = \mathtt{Datum}$. The second new functional parameter is calculated using:

$$D_{Mean,Tube} = \frac{D_{Ext,Tube} + D_{Int,Tube}}{2}, \tag{18}$$

with the simple relations $D_{Ext,Tube} = \texttt{Datum}$ and $D_{Int,Tube} = \texttt{Datum}$ for the new functional parameters. The third new functional parameter is also a datum, taken from the level controller of the humidifier, i.e., $L_{Efec,Tube} = \texttt{Datum}$.
For the other new functional parameter produced by Eq. (16), the used expression is taken from [2], i.e.,

$$M'_{wv} = K_M \left(CW_{Mem,W} - CW_{Mem,Air} \right), \tag{19}$$

being the new functional parameters: K_M the mass transfer overall coefficient, and $CW_{Mem,W}$ and $CW_{Mem,Air}$ the water-side and air-side water concentration of the Nafion membrane, respectively. Each parameter has a function to evaluate its value as it is shown below in Table 4.

B. Friction energy losses $h_{f_{i\to i+1}}$: the losses are evaluated in accordance to the mechanical characteristic and material of the section being considered, i.e., straight line or fitting. The total losses are the sum of individual losses in all straight tubes and their fittings, that is:

$$h_{f_{i\to i+1}} = \sum_j h_{f_{tube,j}} + \sum_k h_{f_{fitting,k}}, \tag{20}$$

where j and k are indices for sections and fitting, respectively. Besides, $j+k$ new functional parameters appear, which are $h_{f_{tube,j}}$ and $h_{f_{fitting,k}}$. For the energy losses in tube straight lines $h_{f_{tube,j}}$, the Darcy-Weisbach equation is used as

$$h_{f_{tube,j}} = f_D \frac{L}{D} \frac{v_j^2}{2}, \tag{21}$$

being f_D the Darcy friction factor calculated using the Shacham equation [7]. Moreover, L_j and D_j are the length and internal diameter of the tube in j-th section, respectively. These parameters have constant value from the assembly scheme. Besides, v_j is the velocity of the mixture into the tube, parameter evaluated using:

$$v_j = \frac{\dot{m}_j \frac{1}{\overline{\rho}_a}}{A_{F,j}}, \tag{22}$$

where $\dot{m}_j$ and $A_{F,j}$ are mass flow rate and the flow area of the j-th tube or straight section, respectively. Besides, $\overline{\rho}_a$ is the mean density of the mixture. The flow area is calculated with the well-known formula for a circle area:

$$A_{F,j} = \frac{\pi D_j^2}{4}.$$

Regarding the energy losses in fittings $h_{f_{fitting,k}}$, the following expression is used:

$$h_{f_{fitting,k}} = K_{F_k} \frac{v^2}{2}, \tag{23}$$

where K_{F_k} is the friction factor of the fitting, which is evaluated with the $2K$ method proposed by Hooper [8], i.e.,

$$K_{F_k} = \frac{K_1}{N_{Re}} + K_\infty \left(1 + \frac{1}{ID_k}\right), \tag{24}$$

being K_1 and K_∞ both constants associated to each kind of fitting and reported by Hooper in his work [8]. Moreover, ID_k is the internal diameter of the fitting (in inches), taken equal to the internal diameter of the straight tube of less internal diameter connected to the fitting. Finally, N_{Re} is the Reynolds number evaluated at the fitting flow conditions, i.e.,

$$N_{Re} = \frac{\rho_a \, v_j \, D_j}{\mu_a}, \tag{25}$$

where μ_a is the viscosity of the mixture evaluated as it is presented below in Table 4.

To avoid lengthening this document and making it tedious, the deduction procedure for the rest of model parameters is not presented in this supplementary material, but all expressions or values for each structural or functional parameter of the model are outlined in Table 4, following the sequence used during the deduction of the model extended structure. This sequence is the same as the one stated for structural parameters in Table 2.

Table 4: Constitutive and assessment equations for model parameters. Subscripts i are for streams and j for assembly sections.

Description	**Constitutive/assessment equation**	**Units**
Mass flow of the fed mixture	$\dot{m}_0 = \mathtt{Datum}$	$\frac{\mathrm{kg}}{\mathrm{s}}$
Density of the mixture	$\rho_{a,i} = \frac{P_i}{R\,T_i}\,\mathfrak{M}_{da}\left[1 - y_{wv,i}\left(1 - \frac{\mathfrak{M}_{wv}}{\mathfrak{M}_{da}}\right)\right]$	$\frac{\mathrm{kg}}{\mathrm{m}^3}$
Pressure at assembly inlet	$P_0 = \mathtt{Datum}$	Pa
Temperature of fed mixture	$T_0 = \mathtt{Datum}$	K
Molar fraction of water vapour in the mixture	$y_{wv,i} = w_{wv,i}\frac{\mathfrak{M}_{da}}{\mathfrak{M}_{wv}}$	$\frac{\text{kmol water}}{\text{kmol a}}$
Mass fraction of vapour in fed mixture	$w_{wv,4} = \mathtt{Datum}$	$\frac{\text{kmol water}}{\text{kmol}}$
Friction energy losses	$h_{f_{i\to i+1}} = \sum_j h_{f_{tube\,j}} + \sum_k h_{f_{fitting\,k}}$	$\frac{\mathrm{m}^2}{\mathrm{s}^2}$
Tube straight line losses	$h_{f_{tube\,j}} = f_D\,\frac{L_j}{D_j}\,\frac{v_j^2}{2}$	$\frac{\mathrm{m}^2}{\mathrm{s}^2}$
Darcy friction factor [7]	f_D: Shacham	—

... This table continues in the next page.

Description	**Constitutive/assessment equation**	**Units**
Length of the tube	$L_j = \mathtt{Datum}$	m
Internal Diameter of the tube	$D_j = \mathtt{Datum}$	m
Mixture velocity into the tube	$v_j = \frac{\dot{m}_j \frac{1}{\rho_a}}{A_{F,j}}$	$\frac{\text{m}}{\text{s}}$
Flow area of the tube	$A_{F,j} = \frac{\pi D_j^2}{4}$	m^2
Energy losses in fittings	$h_{f_{fitting\,k}} = K_{F_k} \frac{v_j^2}{2}$	$\frac{\text{m}^2}{\text{s}^2}$
Friction factor of the fitting [8]	$K_{F_k} = \frac{K_1}{N_{Re}} + K_\infty \left(1 + \frac{1}{ID_k}\right)$	—
Flow fitting constant [8]	$K_1 = \mathtt{Datum}$	—
Reynolds number	$N_{Re} = \frac{\rho_a v_j D_j}{\mu_a}$	—
Viscosity of the mixture	$\mu_a = \frac{y_{da}\,\mu_{da}}{y_{da}+y_{wv}\,\Phi_{da-wv}} + \frac{y_{wv}\,\mu_{wv}}{y_{wv}+y_{da}\,\phi_{wv-da}}$	$\frac{\text{kg}}{\text{m s}}$
Dry air viscosity	$\mu_{da} = 10^{-6}\Big(-9.8601\times10^{-1} + 9.08012\times10^{-2}T - 1.17635575\times10^{-4}T^2 + 1.2349703\times10^{-7}T^3 - 5.7971299\times10^{-11}T^4\Big)$	$\frac{\text{kg}}{\text{m s}}$
Vapour viscosity	$\mu_{wv} = 10^{-6}\left(80.581318 + 4.000549\times10^{-1}T\right)$	$\frac{\text{kg}}{\text{m s}}$
Air-Vapour correction	$\Phi_{da-wv} = \xi_a \left[1 + \left(\frac{\mu_{da}}{\mu_{wv}}\right)^{\frac{1}{2}} \left(\frac{\mathfrak{M}_{wv}}{\mathfrak{M}_{da}}\right)^{\frac{1}{4}}\right]^2$ with $\xi_a = \frac{\sqrt{2}}{4}\left(1 + \frac{\mathfrak{M}_{da}}{\mathfrak{M}_{wv}}\right)^{-\frac{1}{2}}$	—
Vapour-Air correction	$\Phi_{wv-a} = \xi_b, \left[1 + \left(\frac{\mu_{wv}}{\mu_{da}}\right)^{\frac{1}{2}} \left(\frac{\mathfrak{M}_{da}}{\mathfrak{M}_{wv}}\right)^{\frac{1}{4}}\right]^2$ with $\xi_b = \frac{\sqrt{2}}{4}\left(1 + \frac{\mathfrak{M}_{wv}}{\mathfrak{M}_{da}}\right)^{-\frac{1}{2}}$	—
Size fitting constant [8]	$K_\infty = \mathtt{Datum}$	—
Internal diameter of tube in inches	$ID_K = 39.37\, D_K$	m
Mass flow from humidifier	$\dot{m}_5 = \dot{m}_4 + \dot{m}_8$	$\frac{\text{kg}}{\text{s}}$
Mass flow at humidifier inlet	$\dot{m}_4 = \dot{m}_0$	$\frac{\text{kg}}{\text{s}}$
Water vapour flow due by mass transfer	$\dot{m}_8 = A_M\, M'_{wv}$	$\frac{\text{kg}}{\text{m}^2\text{s}}$
Mass transfer area	$A_{Mem} = N_{NT}\left(\pi\, D_{Mean,Tube}\, L_{Efec,Tube}\right)$	m^2
Number of Nafion tubes into the humidifier	$N_{NT} = 1100$	—
Mean diameter of a Nafion tube	$D_{Mean,Tube} = \frac{(D_{Int,Tube}+D_{Ext,Tube})}{2}$	m

... This table continues in the next page.

Description	Constitutive/assessment equation	Units
Effective length of a Nafion tube	$L_{Efec,Tube} = \texttt{Datum}$	m
Mass transfer flux of water vapour [2]	$M'_{wv} = K_M\,(CW_{Mem,W} - CW_{Mem,Air})$	$\frac{\text{kg}}{\text{m}^2\text{s}}$
Overall mass transfer coefficient [2]	$K_M = \frac{\mathfrak{D}_{Mem}}{\epsilon_{Mem}}$	$\frac{\text{m kg}}{\text{s kmol}}$
Diffusivity of water through Nafion membrane	$\mathfrak{D}_{Mem} = \mathfrak{D}_{\lambda_m}^{E_0\left(\frac{1}{303}-\frac{1}{T}\right)}$	$\frac{\text{m}^2}{\text{s}}$
Activation energy for the membrane [2]	$E_0 = 61340.7$	$\frac{\text{J}}{\text{mol}}$
Intra-diffusion coefficient	$\mathfrak{D}_{\lambda_m} = \begin{cases} 10^{-1} & \text{if } \lambda_m < 2 \\ (1+2(\lambda_m-2))\times 10^{-6} & \text{if } 2 \geq \lambda_m \geq 3 \\ (3-1.67(\lambda_m-3))\times 10^{-6} & \text{if } 3 \geq \lambda_m < 4.5 \\ 1.25\times 10^{-6} & \text{if } \lambda_m \geq 4.5, \end{cases}$	$\frac{\text{m}^2}{\text{s}}$
Membrane humidity coefficient	$\lambda_m = 36\,(RH_{Mem})^3 - 39.85\,(RH_{Mem})^2 + 17.81\,RH_{Mem} + 0.043$	—
Mean relative humidity at membrane	$RH_{Mem} = \frac{RH_5 + RH_{\text{water side}}}{2}$	—
Relative humidity air	$RH_i = \frac{y_{wv,i}}{y^*_{wv,i}}$	—
Air humidity at saturation [6]	$y^*_{wv,i} = \frac{P_{Vap,i}}{P_i}$	—
Vapour pressure at saturation [4]	$P_{Vap,i} = Antoine$	Pa
Relative humidity water side	$RH_{\text{water side}} = 1.0$	—
Membrane thickness	$\epsilon_{Mem} = 133.5$	μ m
Water molar-volumetric concentration on membrane at water-side	$CW_{Mem,W} = 28.3636$	$\frac{\text{kmol}}{\text{m}^3}$
Water molar-volumetric concentration on membrane at air-side	$CW_{Mem,Air} = \frac{\rho_{Mem,S}}{\mathfrak{M}_{Mem,S}}\,\lambda_m$	$\frac{\text{kmol}}{\text{m}^3}$
Mass fraction of water vapour	$w_{w,i} = y_{wv,i}\,\frac{\mathfrak{M}_w}{\mathfrak{M}_{da,5}}$	$\frac{\text{kg w}}{\text{kg a}}$
Molar fraction of water vapour at humidifier inlet	$y_{wv,4} = y_{w,0} = \texttt{Datum}$	$\frac{\text{kmol w}}{\text{kmol a}}$
Molar mass of humid air at humidifier outlet	$\mathfrak{M}_{da,5} = y_{wv,5}\,\mathfrak{M}_w + (1 - y_{wv,5})\,\mathfrak{M}_{da}$	$\frac{\text{kg}}{\text{kmol}}$
Change of mass into PS_V	$\Delta M_{PS_V} = \dot{m}_4 - \dot{m}_5 + \dot{m}_8$	$\frac{\text{kg}}{\text{s}}$

... This table continues in the next page.

Description	Constitutive/assessment equation	Units
Heat capacity at constant volume of humid air at humidifier exit	$\widehat{C}_{V_{a,i}} = \widehat{C}_{P_{a,i}} - R_{da}$	$\frac{\text{kJ}}{\text{kg K}}$
Heat capacity at constant pressure of humid air at humidifier exit	$C_{P_{a,i}} = C_{P_{da}} \left(1 - y_{wv,i}\right) \dfrac{\mathfrak{M}_{da}}{\mathfrak{M}_v} + C_{P_{wv}}\, y_{wv,i}\, \dfrac{\mathfrak{M}_{wv}}{\mathfrak{M}_{da}}$	$\frac{kJ}{kg-K}$
Heat capacity at constant pressure of dry air [6]	$C_{P_{da}} = 0.1077024 \times 10^{-12}\, T^4 - 0.4970786 \times 10^{-9}\, T^3 + 0.7816818 \times 10^{-6}\, T^2 - 0.284887 \times 10^{-3}\, T + 1.03409$ with T in degrees Celsius	$\frac{\text{kJ}}{\text{kg K}}$
Heat capacity at constant pressure of water vapour [6]	$C_{P_{wv}} = 1.941058941 \times 10^{-5}\, T^2 - 2.578421578\, 10^{-4}\, T + 1.86910989$ with T in degrees Celsius	$\frac{\text{kJ}}{\text{kg K}}$
Ideal gas universal constant for dry air	$R_{da} = \frac{R}{\mathfrak{M}_{da}}$	
Heat flow from Nafion tubes to air into humidifier	$\dot{Q}_{T-A} = \mathtt{Datum}$	$\frac{\text{kJ}}{\text{s}}$
Pressure drop into humidifier [9]	$\Delta_{P_{4\to5}} = 1.2597 \times 10^8\, \dot{V}_a$	Pa
Liquid water specific heat capacity	$\widehat{C}_{P_{Wl}} = 4.184$	$\frac{\text{kJ}}{\text{kg}^\circ\text{C}}$
Liquid water mass into humidifier	$M_{PS_{VI}} = \mathtt{Datum}$	m^3
Heat flow from Heater to liquid water into humidifier	$\dot{Q}_{H1-W} = \mathtt{Datum}$	$\frac{\text{kJ}}{\text{s}}$
Lost heat from humidifier	$\dot{Q}_{Lost} = \mathtt{Datum}$	$\frac{\text{kJ}}{\text{s}}$
Mass into last section	$M_{PS_{VII}} = V_{PS_{VII}}\, \rho_{a,6}$	kg
Volume of last section	$V_{PS_{VII}} = L_{5-6}\, \frac{\pi D_{5-6}^2}{4}$	m^3
Length of last section	$L_{5-6} = \mathtt{Datum}$	m
Diameter of tube of last section	$D_{5-6} = \mathtt{Datum}$	m
Heat flow from heater to air into last section	$\dot{Q}_{H2-A} = \mathtt{Datum}$	$\frac{\text{kJ}}{\text{s}}$

References

1. D. Green, R. Perry, Chemical Engineering Handbook, eighth ed., McGraw-Hill, New York, USA, 2008.
2. Solsona, M., Kunusch, C., Ocampo, C.: Control-oriented model of a membrane humidifier for fuel cell applications. Energy Convers. Manag. (2017) doi: https://doi.org/10.1016/j.enconman.2017.01.036
3. M. Schoen, The Joule-Thompson effect in confined fluids, Physica A 270 (3) (1999) 353–379, http://dx.doi.org/10.1016/S0378-4371(99)00189-2.
4. J. Seader, E. Henley, D. Roper, Separation Process Principles. Chemical and Biochemical Operations, John Wiley and Sons. Inc., New York, NY, USA, 2011.
5. L. Ljung, System Identification: Theory for the User, Prentice Hall Inc., New Jersey, USA, 1999.
6. D. Green, R. Perry, Chemical Engineering Handbook, eighth ed., McGraw-Hill, New York, USA, 2008.
7. B.J. Schorle, S.W. Churchill, M. Shacham, Comments on: An explicit equation for friction factor in pipe, Ind. Eng. Chem. Fundam. 19 (2) (1980) 228, http://dx.doi.org/10.1021/i160074a019.
8. W.B. Hooper, The two k method predics head losses in pipe and fittings, Chem. Eng. (1981) 96–100.
9. A. Cellkraft, Cellkraft Flow-through humidifiers, Stockholm, Sweden, 2022, URL https://www.cellkraft.se/downloads/P-Series.pdf.