COMSOL Equation Environment

Domain Transport (unknown dependent variable u) $e_{a}\frac{\partial^{2}\boldsymbol{u}}{dt^{2}} + d_{a}\frac{\partial\boldsymbol{u}}{\partial t} + \nabla \cdot (-c \cdot \nabla \boldsymbol{u} - \alpha \boldsymbol{u} + \gamma) + \beta \cdot \nabla \boldsymbol{u} + a\boldsymbol{u} = f$

Boundary flux $-\boldsymbol{n} \cdot (-c \cdot \nabla \boldsymbol{u} - \alpha \boldsymbol{u} + \gamma) = g - q\boldsymbol{u}$

Adsorption and Diffusion inside Desiccant Material

Governing Equations

Air Domain

$$\begin{cases} c_a \rho_a \frac{\partial T}{\partial t} + c_a \rho_a \left(u_x \frac{\partial T}{\partial x} + u_y \frac{\partial T}{\partial y} \right) = 0\\ \rho_a \frac{\partial Y}{\partial t} + \rho_a \left(u_x \frac{\partial T}{\partial x} + u_y \frac{\partial Y}{\partial y} \right) = 0 \end{cases}$$

Desiccant Domain

$$\begin{cases} \rho_m c_d \frac{\partial T}{\partial t} = k_d \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} \right) + q_{ads} \rho_d \frac{\partial W}{\partial t} \\ \epsilon \rho_a \frac{\partial Y}{\partial t} + \rho_d \frac{\partial W}{\partial t} = \rho_a D_A \left(\frac{\partial^2 Y}{\partial x^2} + \frac{\partial^2 Y}{\partial y^2} \right) + \rho_d D_S \left(\frac{\partial^2 W}{\partial x^2} + \frac{\partial^2 W}{\partial y^2} \right) \\ \frac{W}{W_{max}} = \frac{\phi}{R + (1 - R)\phi} \Leftrightarrow \phi = \frac{R \cdot W}{W_{max} - (1 - R) \cdot W} \end{cases}$$

COMSOL Implementation

Using one PDE-module for the heat transfer and one with two equation sets for the mass transfer, the set of equations can be resembled exactly in the form above, with an additional statement in the air domain forbidding the transport of adsorbed species.

Heat Transfer

$$e_{a} = 0, \ \alpha = 0, \ \gamma = 0, \ a = 0, \ d_{a} = \begin{pmatrix} c_{a}\rho_{a} & 0\\ 0 & \rho_{m}c_{d} \end{pmatrix}, \ c = \begin{pmatrix} 0 & 0\\ 0 & k_{d} \end{pmatrix}, \ \beta = \begin{pmatrix} \vec{u} & 0\\ 0 & 0 \end{pmatrix}$$
$$\begin{cases} c_{a}\rho_{a}\frac{\partial T}{\partial t} + c_{a}\rho_{a}\left(u_{x}\frac{\partial T}{\partial x} + u_{y}\frac{\partial T}{\partial y}\right) = 0\\ \rho_{m}c_{d}\frac{\partial T}{\partial t} - k_{d}\left(\frac{\partial^{2}T}{\partial x^{2}} + \frac{\partial^{2}Y}{\partial y^{2}}\right) = 0 \end{cases}$$

Mass Transfer (in the Air)

 $e_a=0,\ c=0,\ \alpha=0,\ \gamma=0,\ a=0,\ d_a=\begin{pmatrix}\rho_a&0\\0&1\end{pmatrix},\ \beta=\begin{pmatrix}\vec{u}&0\\0&0\end{pmatrix}$

$$\begin{cases} \rho_a \frac{\partial Y}{\partial t} + \rho_a \left(u_x \frac{\partial T}{\partial x} + u_y \frac{\partial Y}{\partial y} \right) = 0\\ \frac{\partial W}{\partial t} = 0 \end{cases}$$

Mass Transfer (in the Desiccant) $e_a = 0, \ \alpha = 0, \ \gamma = 0, \ \beta = 0,$

$$d_{a} = \begin{pmatrix} \epsilon \rho_{a} & \rho_{d} \\ 0 & 0 \end{pmatrix}, \quad c = \begin{pmatrix} \rho_{a} D_{A} & \rho_{d} D_{S} \\ 0 & 0 \end{pmatrix}, \quad a = \begin{pmatrix} 0 & 0 \\ 0 & (W_{max})^{-1} \end{pmatrix}, \quad f = \begin{pmatrix} 0 & 0 \\ \phi (R + (1 - R)\phi)^{-1} \end{pmatrix}$$
$$\begin{cases} \epsilon \rho_{a} \frac{\partial Y}{\partial t} + \rho_{d} \frac{\partial W}{\partial t} = \rho_{a} D_{A} \left(\frac{\partial^{2} Y}{\partial x^{2}} + \frac{\partial^{2} Y}{\partial y^{2}} \right) + \rho_{d} D_{S} \left(\frac{\partial^{2} W}{\partial x^{2}} + \frac{\partial^{2} W}{\partial y^{2}} \right) \\ \frac{W}{W_{max}} = \frac{\phi}{R + (1 - R)\phi}$$

Results

Model fails to converge for simulation times greater than 10s. Close to the boundary, there is transport of adsorbed species into the air stream.

