A machine learning based model for membrane-based absorbers in absorption heat pumps

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Abstract

A new multi-label machine learning-based model is proposed for membrane-based absorbers used in absorption heat pumps and chillers. The model offers the accuracy of a numerical model with the computational efficiency of an analytical model. A comprehensive dataset, comprising of 100,000 data points, is generated using 2D numerical modeling. The dataset consists of 15 input parameters, including operating conditions and geometrical parameters, and four output variables including absorption rate, outlet concentration, solution outlet temperature, and heat transfer fluid outlet temperature. Support Vector Regressor, Random Forest Regressor, and Decision Tree Regressor algorithms are used to develop the present model. The results of the proposed model are validated with the experimental data available in the literature, capturing the trend of the data with a relative difference of 15%. It is shown that the present machine learning-based model can predict the four outputs with an accuracy of over 90%.

Keywords: machine learning; absorption chillers and heat pumps; membrane-based absorber; heat and mass transfer; and membrane technology.

1. Introduction

Several studies have been conducted to analyze a membrane-based absorber's performance using computational fluid dynamics (CFD) and other numerical methods [1–4]. These methods can produce detailed results; however, implementing such models incurs a high computational cost. Analytical models [5,6] offer efficient computation, but they may have limiting assumptions such as isothermal boundary condition at the heat exchanger wall. As such, they cannot consider the temperature lift and heat exchanger wall thickness.

There are only a few studies on membrane-based absorbers that use machine learning, and they are generally for minimizing flow maldistribution in membrane-based absorbers [7], geometry optimization [8], or investigating the available ionic liquid absorbents for absorption heat pumps [9]. In this study, we propose a new multi-label machine learning-based model for membrane-based absorbers used in absorption chillers and heat pumps for the first time. A multi-label machine learning model enables predicting more than one independent variable. A comprehensive dataset, comprising of 100,000 data points, is generated using our 2D numerical model, which was run on Compute Canada's supercomputers, namely, Narval, Cedar, Graham, and Beluga [10].

2. Problem description

Coupled heat and mass transfer in membrane-based absorbers is numerically studied for two configurations: i) the single-sided configuration, where the absorption heat is transferred to the heat transfer fluid only from one side, shown in Fig. 1(a); and ii) the double-sided configuration,

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in which the absorption heat is transferred to the heat transfer fluid from both sides, shown in Fig. 1(b). Lithium bromide-water is used as the solution, which is the most common absorbent in absorption chillers/heat pumps. The liquid solution is constrained by a microporous/nanofibrous membrane and a plate heat exchanger. The membrane is impermeable to the LiBr-water solution, while water vapor can traverse the membrane leading to water vapor absorption at the membrane-solution interface.

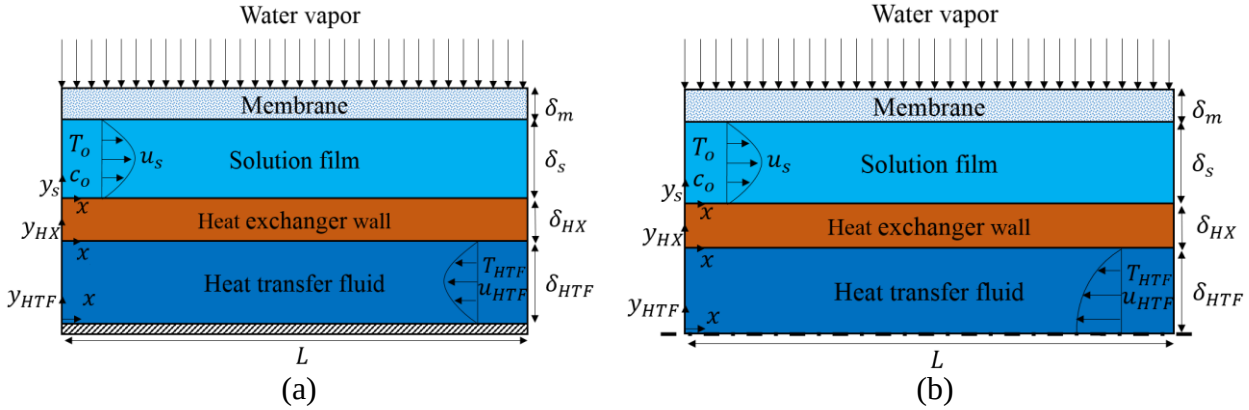

Fig. 1. A schematic diagram of a membrane-based absorber over a heat exchanger. (a) the single-sided configuration; and (b) the double-sided configuration (symmetry boundary condition is applied).

3. Model development

The following governing equations for energy and species conservation can be derived for the advective transport in the flow direction x and diffusivity transport in the y_s direction for the solution domain:

$$u_s \frac{\partial T_s}{\partial x} = \alpha_s \frac{\partial^2 T_s}{\partial y_s^2} \quad (1)$$

$$u_s \frac{\partial c_s}{\partial x} = D_s \frac{\partial^2 c_s}{\partial y_s^2} \quad (2)$$

where, T, α_s, c_s and D_s are the solution's temperature, thermal diffusivity, concentration, and mass diffusivity, respectively. Energy equations for the heat transfer fluid and heat exchanger wall can be written as follows:

$$u_{HTF} \frac{\partial T_{HTF}}{\partial x} = \alpha_{HTF} \frac{\partial^2 T_{HTF}}{\partial y_{HTF}^2} \quad (3)$$

$$\frac{\partial^2 T_{HX}}{\partial y_{HX}^2} + \frac{\partial^2 T_{HX}}{\partial x^2} = 0 \quad (4)$$

where, T_{HTF}, α_{HTF}, and T_{HX} are the heat transfer fluid's temperature, thermal diffusivity, and heat exchangers' temperature, respectively. The Dusty-Gas model [11] is used to model the mass transfer through the membrane:

$$J = k_m(p_v - p_{inf}) \quad [\frac{kg}{m^2.s}] \quad (5)$$

where, k_m, p_v, and p_{inf} are the membrane mass transfer coefficient, vapor pressure, and water vapor partial pressure at the membrane-solution interface, respectively. The governing equations should be solved simultaneously and iteratively. A finite difference method was used to solve the governing equations. The first and second derivatives of the parameters were discretized using a central difference method. Virtual nodes were considered to couple the boundary conditions to

the domain to maintain second-order accuracy. All the equations were solved iteratively until a residual of 10^{-8} was reached for each parameter. Thermophysical properties for the solution and the heat transfer fluid were calculated at each iteration, more details can be found in Ref [12]. Computations were performed on Compute Canada's supercomputers, namely, Narval, Cedar, Graham, and Beluga [10].

4. Machine learning process

4.1. Data description

This study generated a dataset, comprising of 100,000 data, using our 2D numerical model for a membrane-based absorber. The dataset includes 15 features, which are the input parameters in a machine learning model, including operating conditions and geometrical parameters listed in Table 1. There are 4 labels, which are the selected output parameters of the model, including absorption rate, outlet concentration, solution outlet temperature, and heat transfer fluid outlet temperature. The range for the selected features has been picked to cover all practical operating conditions and geometrical parameters of an actual absorption setup available in the literature [13–15] to ensure usability of the present machine learning-based model.

Table 1- The features' ranges used for the current machine learning-based model.

Feature name	**Feature type**	**Feature range**	**Available experimental range in the literature** [13–15]
Absorber length $\boldsymbol{L}$ $[\boldsymbol{cm}]$	Numeric	$1-10$	$3-5$
Solution thickness $\boldsymbol{\delta_s}$ $[\boldsymbol{\mu m}]$	Numeric	$50-500$	$100-200$
Average solution velocity $\boldsymbol{\bar{u}_s}$ $[\frac{\boldsymbol{mm}}{\boldsymbol{s}}]$	Numeric	$0.1-20$	$5-15$
Solution inlet temperature $\boldsymbol{T_o}$ $[\boldsymbol{^oC}]$	Numeric	$25-55$	$25-35$
Water inlet concentration $\boldsymbol{c_o}$ $[\frac{\boldsymbol{kg\ water}}{\boldsymbol{kg\ solution}}]$*	Numeric	$0.38-0.55$	$0.4-0.45$
Heat transfer fluid inlet temperature $\boldsymbol{T_{HTF}}$ $[\boldsymbol{^oC}]$	Numeric	$25-55$	$25-30$
Vapor pressure $\boldsymbol{p_v}$ $[\boldsymbol{kPa}]$	Numeric	$0.840-2.34$	$0.840-1.9$
Membrane porosity $\boldsymbol{\varphi}$	Numeric	$0.1-1$	$0.4-0.9$
Membrane pore diameter $\boldsymbol{D_m}$ $[\boldsymbol{\mu m}]$	Numeric	$0.2-3$	$0.45-1$
Membrane thickness $\boldsymbol{\delta_m}$ $[\boldsymbol{\mu m}]$	Numeric	$10-250$	$50-150$
Heat exchanger wall thickness $\boldsymbol{\delta_{HX}}$ $[\boldsymbol{mm}]$	Numeric	$0.5-5$	N/A
Heat transfer fluid thickness $\boldsymbol{\delta_{HTF}}$ $[\boldsymbol{mm}]$	Numeric	$0.25-5$	$0.25-5$
Heat exchanger thermal conductivity $\boldsymbol{k_{HX}}$ $[\frac{\boldsymbol{W}}{\boldsymbol{m.K}}]$	Numeric	13-17 Stainless steel 170-230 Aluminum	Both
Average heat transfer fluid velocity $\boldsymbol{\bar{u}_{HTF}}$ $[\frac{\boldsymbol{mm}}{\boldsymbol{s}}]$	Numeric	$0.1-20$ Parallel flow $-0.1\ to-20$ Counter flow	N/A
Configuration	Binary	0 single-sided configuration 1 double-sided configuration	Single-sided configuration

* Water concentration $c_o = 1 - X$ where X is the solution concentration.

4.2. Machine learning-based model development

The Support Vector Regressor (SVR) [16], Random Forest Regressor (RFR) [17], and Decision Tree Regressor (DTR) [18] are implemented and combined to improve the model's accuracy. 90% of the dataset is used for training, and 10% is used for testing. Figure 2 shows the predicted label versus the actual label based on the numerical modeling. The following can be observed: i) the absorption rate can be predicted with an accuracy of 90%; ii) the outlet

concentration can be predicted with an accuracy of 98%; and iii) the solution outlet temperature and heat transfer fluid outlet temperature can be predicted with an accuracy of ± 99.5%.

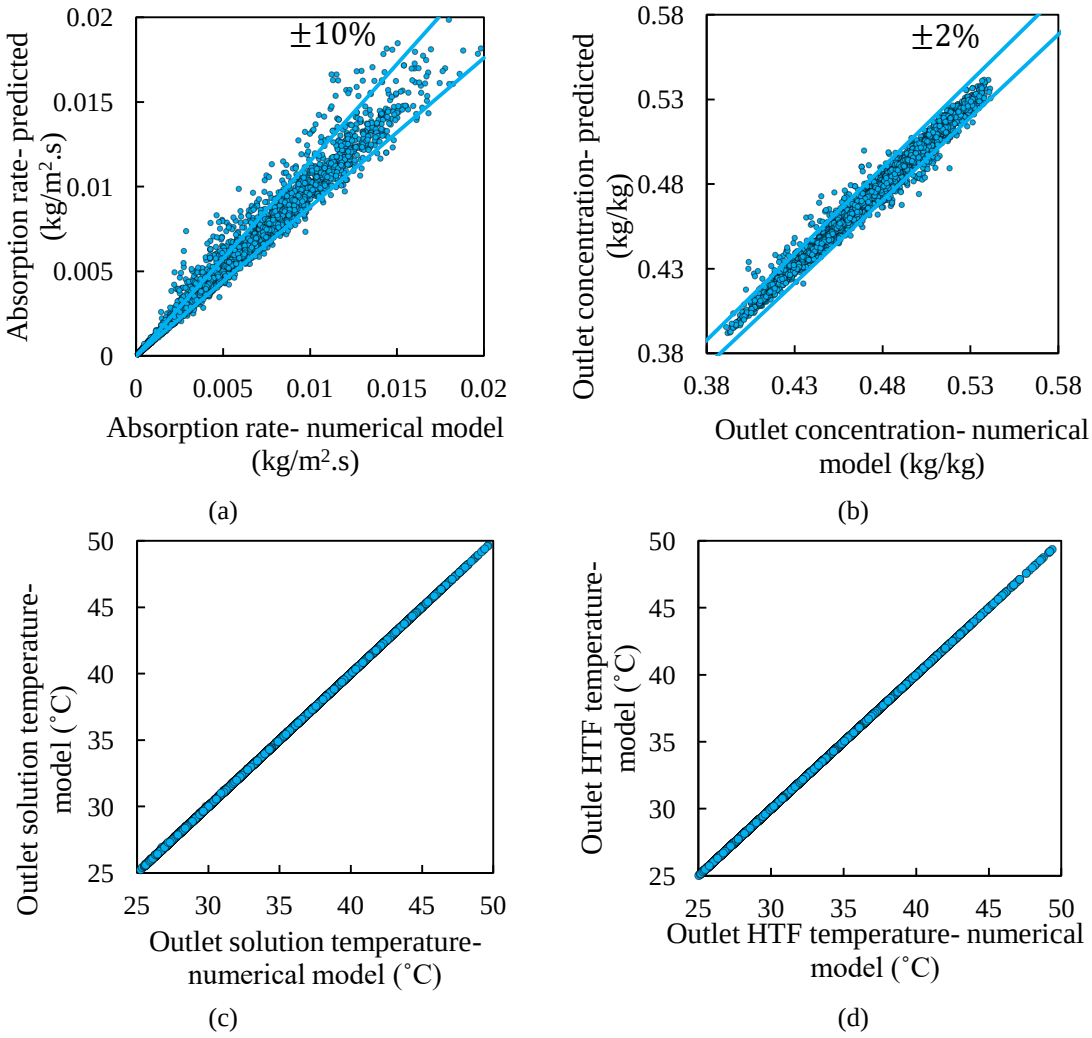

Fig. 2. The predicted label versus the actual label based on numerical modeling for the present labels.

4.3.Validation with experimental data

The machine learning model is validated with experimental data from Isfahani et al. [13,14]. As shown in Fig. 3, the present model can predict the experimental data, capturing data within a relative difference of 15%.

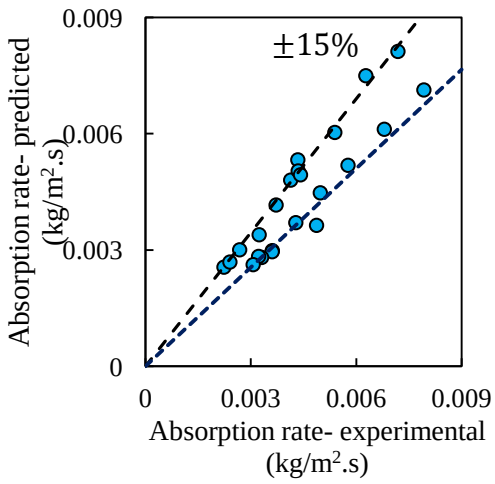

Fig. 3. Validation of the present machine learning based model with experimental data from Refs. [13,14].

Conclusion

In this study, we proposed a multi-label machine learning-based model for membrane-based absorbers used in absorption heat pumps and chillers for the first time. The generated dataset, comprising of 100,000 data, consists of 15 input parameters, including operating conditions and geometrical parameters, and four output variables, i.e., the

absorption rate, outlet concentration, solution outlet temperature, and heat transfer fluid outlet temperature. The results of the machine learning-based model were validated with experimental data.

Supplementary data

The present machine learning model and dataset are shared on GitHub, enabling prospective readers to perform real-time absorber control, optimization, and design in an accurate, time-efficient manner.

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