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Fast, stable computation of thermodynamic properties of ammonia-water mixtures

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ABSTRACT

Software implementations of thermodynamic property routines for ammonia-water mixtures are developed for refrigeration and air-conditioning applications. Saturation correlations are employed to identify single-phase state points, yielding up to a 5-fold reduction in property evaluation time. A run-time database of previously evaluated state points is implemented to improve initial guesses for iterative property evaluation, reducing property evaluation time by 45% in a representative study. The property routines are implemented in a standalone program and as a compiled routine for use in MATLAB® and Simulink®. Both implementations perform property evaluations significantly faster than existing software packages. Program performance is measured on a 2.2 GHz machine, and average individual state point evaluation times were found to range from 50 to 930 μs, depending on the provided input properties. Additionally, a segmented, transient, ammonia-water absorber model is developed in Simulink® to assess the use of the property routines for practical engineering calculations. The proposed computational techniques can be applied to accelerate property evaluations for other mixtures.

Etude numérique rapide, stable des propriétés thermodynamiques de mélanges ammoniac-eau

Mots clés : Absorption ; Ammoniac-eau ; Propriétés thermodynamiques ; Mélanges zéotropiques

1. Introduction

1.1. Background

The ammonia-water fluid pair is employed in a broad range of energy systems including absorption refrigeration, heat pumping, and even power generation through the Kalina cycle (Heppenstall, 1998). As these ammonia-water technologies are refined, and specialized two-phase heat and mass exchangers are developed, the demands on thermophysical property formulations, and the software implementations thereof, are greatly increased. The major objectives in the development and implementation of property formulations are outlined below.

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Nomenclature

a, *b*, *c*, *d*	coefficient for empirical property expression [–]
A, *B*, *C*, *D*, *E*, *F*	dimensionless coefficient for empirical property expression [–]
A	heat transfer area, in absorber model [m^2]
c_p	specific heat at constant pressure [kJ kg^{-1} K^{-1}]
E	error at a specific iteration [–]
g	specific Gibbs free energy [kJ kg^{-1}]
h	specific enthalpy [kJ kg^{-1}]
H	total enthalpy, in absorber model [kJ]
J	Jacobian matrix, in iterative solver [–]
k	thermal conductivity [W m^{-1} K^{-1}]
l	segment length, in absorber model [m]
m	segment mass, in absorber model [kg]
$\dot{m}$	mass flow rate, in absorber model [kg s^{-1}]
M	molar mass of mixture [kg $kmol^{-1}$]
P	pressure [kPa]
Q	quality [–]
r	residual vector, in iterative solver [–]
R	gas constant [kJ kg^{-1} K^{-1}]
s	specific entropy [kJ kg^{-1} K^{-1}]
t	time, in absorber model [s]
T	temperature [K]
u	specific internal energy [kJ kg^{-1}]
UA	heat transfer conductance value, in segmented absorber model [W K^{-1}]
v	specific volume [m^3 kg^{-1}]
V	segment volume in absorber model [m^3]
x, *y*	liquid and vapor ammonia mass concentrations [kg kg^{-1}]
$\bar{x}$, $\bar{y}$	liquid and vapor ammonia molar concentrations [kmol $kmol^{-1}$]

Subscripts

0	reference value for saturation correlations, and reference state in absorber model
1,2. . .	coefficient index
a	ammonia
aw	ammonia-water mixture sub-domain of absorber model
B	base value, for computing reduced properties
bub	bubble point (Q = 0, y = 1)
cf	coupling fluid sub-domain of absorber model
DB	value from property database
dew	dew point (Q = 1, *x* = 0)
e, i	. . .inlet/exit. . ., for each fluid segment of the absorber model
E	excess energy, for ammonia-water liquid mixtures
i	specific component (a – ammonia or w – water)
j	segment of discretized absorber model
in	provided input value
m, *n*	exponents in saturation correlations
o	reference dimensionless property
PK	from Pátek and Klomfar saturation correlations
r	reduced, dimensionless property
w	water
w	wall, in absorber model

Superscripts

0	initial guess, for iterative solutions
g	gas phase
j	specific phase (l – liquid or g – gas)
k	current iteration
l	liquid phase