

LA-UR-17-25250

Approved for public release; distribution is unlimited.

Title: Complete Evaluation of Available Laboratory-scale Data for the Independence Model

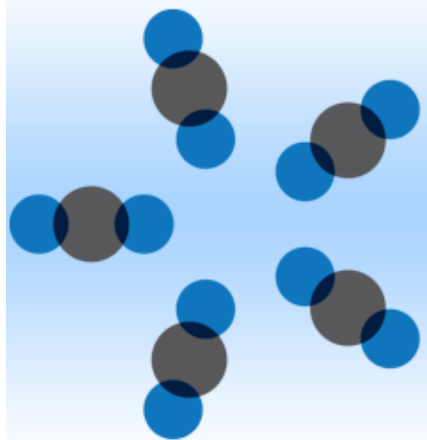
Author(s): Holland, Troy Michael
Kress, Joel David
Bhat, Kabekode Ghanasham

Intended for: Report

Issued: 2017-06-30

Disclaimer:

Los Alamos National Laboratory, an affirmative action/equal opportunity employer, is operated by the Los Alamos National Security, LLC for the National Nuclear Security Administration of the U.S. Department of Energy under contract DE-AC52-06NA25396. By approving this article, the publisher recognizes that the U.S. Government retains nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or to allow others to do so, for U.S. Government purposes. Los Alamos National Laboratory requests that the publisher identify this article as work performed under the auspices of the U.S. Department of Energy. Los Alamos National Laboratory strongly supports academic freedom and a researcher's right to publish; as an institution, however, the Laboratory does not endorse the viewpoint of a publication or guarantee its technical correctness.



CCSI²

Carbon Capture Simulation for Industry Impact

Complete Evaluation of Available Laboratory-scale Data for the Independence Model

Work Performed Under
Activity Number:

Prepared by
Troy Holland
Joel D. Kress
Sham Bhat
Los Alamos National Laboratory

Prepared for
U.S. Department of Energy
National Energy Technology Laboratory

1/31/2017



Revision Log

Revision	Date	Revised By:	Description
0	1/31/2017	Joel D. Kress	Original

Disclaimer

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

Table of Contents

1.0	Preamble	1-1
2.0	Milestone summary and completion	2-1
3.0	Additional information.....	3-1
4.0	Sample Data	4-1
5.0	Acknowledgements.....	5-1
6.0	References.....	6-1

List of Tables

Table 1 - Piperazine(PZ)/Water Heat Capacity Data. x_{PZ} is the mole fraction of Piperazine, x_{H_2O} is the mole fraction of water, and Mixture C_p is the heat capacity of the mixture.	4-2
Table 2 - Volatility Data for PZ in Water. x_{PZ} is the mole fraction of Piperazine and x_{H_2O} is the mole fraction of water.	4-4

1.0 Preamble

Due to waning interest of potential awardees, milestones M1.17.2.B and M1.17.3.B were adjusted. Originally, these milestones read, “Complete evaluation of available laboratory-scale data for Phase 2 awardee #1” (or 2). These milestones were combined to suit the redirected goal of uncertainty quantification (UQ) and calibration of the UT Austin “Independence” model, and now reads, “Complete evaluation of available laboratory-scale data for Independence UQ.”

2.0 Milestone summary and completion

Year 1 Objectives (August 2016 – December 2016) – The original Independence model is a sequentially regressed set of parameters from numerous data sets in the Aspen Plus modeling framework. The immediate goal with the basic data model is to collect and evaluate those data sets relevant to the thermodynamic submodels (pure substance heat capacity, solvent mixture heat capacity, loaded solvent heat capacities, and volatility data). These data are informative for the thermodynamic parameters involved in both vapor-liquid equilibrium, and in the chemical equilibrium of the liquid phase. The data sets for preliminary uncertainty quantification and propagation are:

- Low temperature water/amine heat capacity data (Hilliard, 2008¹)
- High temperature water/amine heat capacity data (Nguyen, 2012²)
- Water/amine volatility data (Hilliard, 2008¹ and Nguyen, 2012²)
- Low temperature CO₂ solubility data (Dugas, 2009³, and Fulks, 2011⁴)
- High temperature CO₂ solubility data (Xu, 2011⁵)
- Loaded CO₂ heat capacity (Freeman, 2010⁶)

3.0 Additional information

The milestone was successfully concluded; additionally the specific inputs, outputs, and parameters relevant for inference for the data were identified and tabulated. This leads directly to model exploration and UQ. Finally, much additional data is likely available, and prime sources have been located. These data are not yet necessary, and will not be mined from past records and literature until future project goals justify the resources necessary to extract the data.

4.0 Sample Data

This section contains sample data needed for the initial calibration and exploration of the thermodynamic submodels critical to UT Austin's modeling effort. The full data sets are extensive, and not detailed here.

Data Table for the Heat Capacity of Piperazine and H₂O

The data below were measured by Dr. Marcus Hilliard in 2008 (UT Austin) using differential scanning calorimetry. They were originally recorded as a portion of his thesis work, with the method fully described on pages 71-87 and the data graphically recorded on page 275.

Table 1 - Piperazine(PZ)/Water Heat Capacity Data. X_{PZ} is the mole fraction of Piperazine, X_{H_2O} is the mole fraction of water, and Mixture C_p is the heat capacity of the mixture.

	TEMPERATURE	PRESSURE	X_{PZ}	X_{H_2O}	Mixture C_p
Units	C	kPa	-	-	kJ/kg-K
STD-DEV	0.1	1%	0.10%	0	3%
	40	101.325	0.0347487	0.965251	3.8677
	45	101.325	0.0347487	0.965251	3.8815
	50	101.325	0.0347487	0.965251	3.8939
	55	101.325	0.0347487	0.965251	3.9053
	60	101.325	0.0347487	0.965251	3.916
	65	101.325	0.0347487	0.965251	3.9258
	70	101.325	0.0347487	0.965251	3.9368
	75	101.325	0.0347487	0.965251	3.9452
	80	101.325	0.0347487	0.965251	3.9591
	85	101.325	0.0347487	0.965251	3.982
	90	101.325	0.0347487	0.965251	3.9996
	95	101.325	0.0347487	0.965251	4.0155
	100	101.325	0.0347487	0.965251	4.03
	105	101.325	0.0347487	0.965251	4.0454
	110	101.325	0.0347487	0.965251	4.0587
	115	101.325	0.0347487	0.965251	4.0721
	120	101.325	0.0347487	0.965251	4.083
	40	101.325	0.060856	0.939144	3.7194
	45	101.325	0.060856	0.939144	3.7304
	50	101.325	0.060856	0.939144	3.7414
	55	101.325	0.060856	0.939144	3.7524
	60	101.325	0.060856	0.939144	3.7634
	65	101.325	0.060856	0.939144	3.7744
	70	101.325	0.060856	0.939144	3.7854
	75	101.325	0.060856	0.939144	3.7964
	80	101.325	0.060856	0.939144	3.8074
	85	101.325	0.060856	0.939144	3.8184
	90	101.325	0.060856	0.939144	3.8294
	95	101.325	0.060856	0.939144	3.8404
	100	101.325	0.060856	0.939144	3.8514
	105	101.325	0.060856	0.939144	3.8624
	110	101.325	0.060856	0.939144	3.8734
	115	101.325	0.060856	0.939144	3.8844
	120	101.325	0.060856	0.939144	3.8954

Sample Volatility Data for PZ/H₂O Solutions

The following data sample was used in the original calibration of Independence (UT Austin's process modeling framework). It is considered to be the most reliable data available for the current system, and was heavily weighted in the initial calibration, and is informative on the Henry's constant for the system. Originally collected by Dr. Bich-Thu Nguyen in 2012 (UT Austin).

Table 2 - Volatility Data for PZ in Water. X_{PZ} is the mole fraction of Piperazine and X_{H_2O} is the mole fraction of water.

	TEMPERATURE	PRESSURE	X_{PZ}	X_{H_2O}
Units	C	N/sqm	-	-
STD-DEV	0.1	4%	1%	0
	50	2.808736	0.034749	0.965251
	60	6.271177	0.034749	0.965251
	70	13.42682	0.034749	0.965251
	50	17.24619	0.125873	0.874127
	55	23.55013	0.125873	0.874127
	60	36.82606	0.125873	0.874127
	65	57.57076	0.125873	0.874127
	70	74.64768	0.125873	0.874127
	55.2	46.46841	0.152541	0.847459
	60	59.67479	0.152541	0.847459
	65	83.99162	0.152541	0.847459
	70.1	145.0694	0.152541	0.847459
	50	2.808736	0.034749	0.965251
	60	6.271177	0.034749	0.965251
	70	13.42682	0.034749	0.965251
	50	2.808736	0.034749	0.965251
	60	6.271177	0.034749	0.965251
	70	13.42682	0.034749	0.965251
	50	17.24619	0.125873	0.874127
	55	23.55013	0.125873	0.874127
	60	36.82606	0.125873	0.874127
	65	57.57076	0.125873	0.874127
	70	74.64768	0.125873	0.874127
	50	17.24619	0.125873	0.874127
	55	23.55013	0.125873	0.874127
	60	36.82606	0.125873	0.874127
	65	57.57076	0.125873	0.874127
	70	74.64768	0.125873	0.874127
	50	17.24619	0.125873	0.874127
	55	23.55013	0.125873	0.874127
	60	36.82606	0.125873	0.874127
	65	57.57076	0.125873	0.874127
	70	74.64768	0.125873	0.874127
	50	17.24619	0.125873	0.874127
	55	23.55013	0.125873	0.874127
	60	36.82606	0.125873	0.874127
	65	57.57076	0.125873	0.874127
	70	74.64768	0.125873	0.874127

5.0 Acknowledgements

We acknowledge Yuan Ye and Prof. Gary Rochelle from the U. of Texas at Austin for valuable discussions and input.

6.0 References

1. Hilliard, M. D. A Predictive Thermodynamic Model for an Aqueous Blend of Potassium Carbonate, Piperazine, and Monoethanolamine for Carbon Dioxide Capture from Flue Gas. UT Austin, Austin, TX, 2008.
2. Nguyen, B.-T. N. Amine Volatility in CO₂ Capture. UT Austin, Austin, TX, 2013.
3. Dugas, R. E. Carbon Dioxide Absorption, Desorption, and Diffusion in Aqueous Piperazine and Monoethanolamine. UT Austin, Austin, TX, 2009.
4. Fulk, S. M. Measuring and Modeling Aerosols in Carbon Dioxide Capture by Aqueous Amines. UT Austin, Austin, Tx, 2016.
5. Xu, Q. Thermodynamics of CO₂ Loaded Aqueous Amines. UT Austin, Austin, Tx, 2011.
6. Freeman, S. A. Thermal Degradation and Oxidation of Aqueous Piperazine for Carbon Dioxide Capture. UT Austin, Austin, TX, 2011.