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

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

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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 quantifiacatin (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, 2008[1])
- High temperature water/amine heat capacity data (Nguyen, 2012[2])
- Water/amine volatility data (Hilliard, 2008[1] and Nguyen, 2012[2])
- Low temperature CO_2 solubility data (Dugas, 2009[3], and Fulks, 2011[4])
- High temperature CO_2 solubility data (Xu, 2011[5])
- Loaded CO_2 heat capacity (Freeman, 2010[6])

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 H_2O

The data below were measured by Dr. Marcus Hilliard in 2008 (UT Austin) using differential scanning calorimetry. They were originially 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_{H2O} is the mole fraction of water, and Mixture C_P is the heat capacity of the mixture.

	TEMPERATURE	PRESSURE	X_{PZ}	X_{H2O}	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/H_2O 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_{H2O} is the mole fraction of water**.**

	TEMPERATURE	PRESSURE	X_{PZ}	X_{H2O}
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
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	50	17.24619	0.125873	0.874127
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	70	74.64768	0.125873	0.874127
	50	17.24619	0.125873	0.874127
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	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.

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