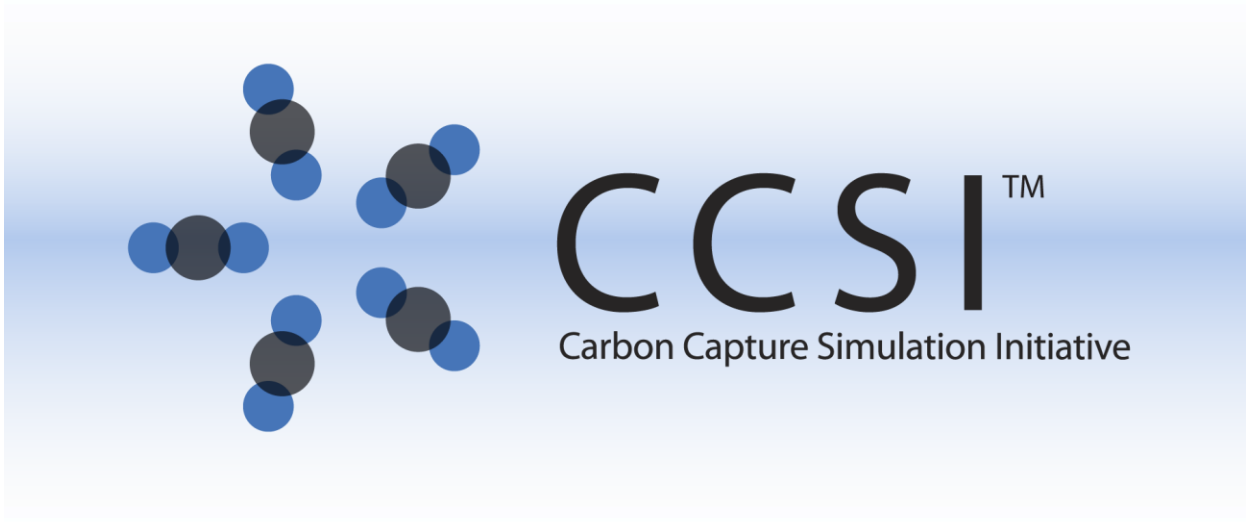

CCSI MEA Dynamic Model (MEA_dm)

User Manual

Version 2.0.0

March 2018

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License Agreement

Table of Contents

List of Figures

List of Tables

To obtain support for the products within this package, please send an e-mail to ccsi-support@acceleratecarboncapture.org.

1.0 REPORTING ISSUES

To report an issue, please send an e-mail to ccsi-support@acceleratecarboncapture.org.

2.0 VERSION LOG

Product	Version Number	Release Date	Description
MEA Dynamic Model	2.0.0	3/31/2018	Initial Open Source release
Steady State MEA Model	2015.10.0	10/16/2015	Initial Release

MEA Dynamic Model

1.0 MODEL BACKGROUND

This document describes the dynamic model of a solvent-based CO_2 capture system using aqueous monoethanolamine (MEA). In addition to this user manual, the download folder consists of the main Aspen Plus® Dynamics® file "CCSI_MEAModel_dynamic.dynf" along with following supporting files:

- EQ_rxnmodified_abs3dyn.appdf
- EQ_rxnmodified_abs3dyn.opt
- EQ_rxnmodified_works.f
- jcm.dll
- jcm.opt

The first supporting file is the properties package obtained from the MEA steady-state process model. The remaining files are related to the FORTRAN user models. This model has been developed with Aspen Plus V8.4. For running the model successfully, all the files should be placed in the same folder.

2.0 GENERAL INFORMATION

Currently, there are very few dynamic models of chemical solvent-based CO_2 capture systems. The existing few dynamic models available in the open literature are validated with a narrow range of operating conditions and for a single step change. As part of the Carbon Capture Simulation Initiative (CCSI), a dynamic model has been developed that has been validated using a wide range of experimental data from the National Carbon Capture Center (NCCC) in Wilsonville, Alabama.

2.1 Overview

This high fidelity "gold standard" steady-state model of the MEA system that has been developed in Aspen Plus as part of CCSI is a rate-based model. However, only equilibrium models are supported in Aspen Plus Dynamics. To get around with this issue, the rate-based model is approximated by using Murphree efficiencies similar to what has been described by Zhang et al.[1] In this work the approach developed by Zhang et al.[1] is further extended and the following correlation is regressed over a wide range of gas and liquid flows and compositions to obtain the Murphree efficiencies:

$$\varepsilon = A\left(\frac{F_L}{F_{Lo}}\right)^{\boldsymbol{B}}\left(\frac{F_V}{F_{Vo}}\right)^{\boldsymbol{C}}\left(\frac{CO_{2\ load}}{CO_{2\ load,o}}\right)^{\boldsymbol{D}}\left(\frac{MEA}{MEA_o}\right)^{\boldsymbol{E}} \quad (1)$$

where, F is the flowrate, $CO_{2\ load}$ is the ratio of mols of CO_2 per mols of MEA in the liquid phase, and MEA is the MEA mass fraction in the liquid phase. The subscript o indicates a reference state of these variables, and the subscripts L and V indicate liquid and vapor phases, respectively. A, B, C, D, and E are parameters regressed to fit the conditions of the column profile using the method of least squares. The equation is then implemented in the equilibrium model in Aspen Plus Dynamics to approximate the rate-based results. Figure 39 shows the comparison between the rate based model and the equilibrium model enhanced with the Murphree efficiency model for CO_2 flowrate from the top of the absorber. In the Aspen Plus Dynamics model, the Murphree efficiency model is implemented as a flowsheet constraint.

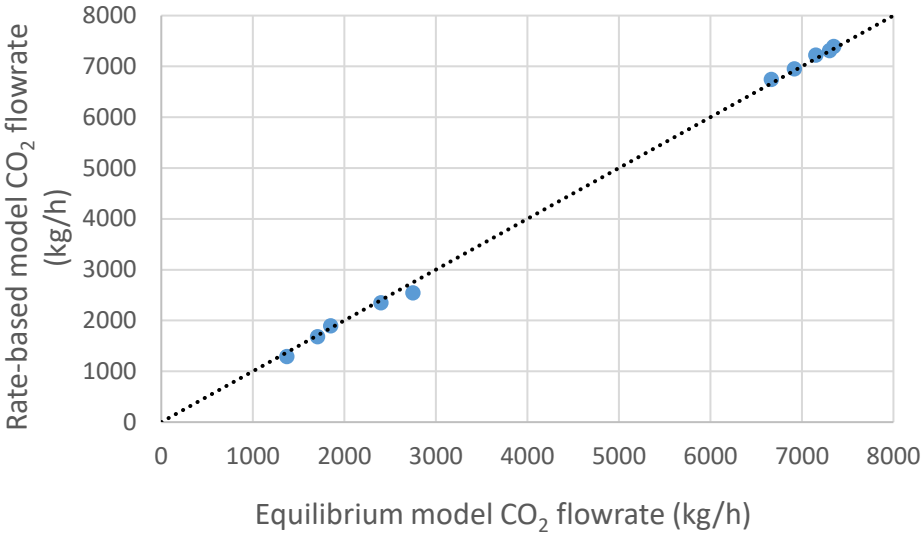

Figure 1: Equilibrium model and rate-based model comparison.

The flowsheet of the dynamic simulation is developed similar to the NCCC pilot plant configuration. Each equipment item is sized using the information from the NCCC pilot plant. This process model includes one flue gas condenser, one buffer tank between the absorber exit and the regenerator inlet, one heat exchanger between rich amine and hot lean amine followed by one cooler for the lean amine, and a lean amine storage tank. The absorber wash tower, the regenerator condenser, and the regenerator reboiler are also included in the flowsheet.

2.2 Thermodynamic Properties Package

This dynamic model is obtained by exporting the steady-state Aspen Plus model developed by CCSI (also part of this release), after converting it to an equilibrium model. Both the Aspen Plus and Aspen Plus Dynamics use Electrolyte-NRTL model in Aspen Properties® as the thermodynamic model.

Additional properties models as described in the User Manual of the Steady State MEA Model and in Morgan et al.,[2] are implemented as FORTRAN user models. The thermodynamic framework of these systems is developed using UT Austin's Phoenix model[3] thermodynamic framework as a precursor. However, the model parameters of the Electrolyte-NRTL models are modified by using heat of absorption data of the ternary MEA-H_2O-CO_2 and binary MEA-H_2O systems and additional VLE data, and heat capacity data. The kinetic model considers the following equilibrium reactions:

$$2MEA + CO_2 \leftrightarrow MEA^+ + MEACOO^- \quad (2)$$

$$MEA + CO_2 + H_2O \leftrightarrow MEA^+ + HCO_3^- \quad (3)$$

The forward reaction rate constants are taken from the Phoenix model, but the overall reaction rate is written in terms of species activities and the equilibrium constants are calculated by using the thermodynamic framework of the system. This follows the methodology presented in Mathias and Gilmartin[4], and is implemented to ensure that the chemical equilibrium is calculated consistently using the thermodynamic model.

2.3 Controllers Configuration

Table 18 provides a list of the controllers in the process flowsheet. The controller's set-points correspond to a typical operating condition in NCCC. Each of these controllers are manually tuned to match the dynamic behavior observed for the collected data.

Table 1: List of Flowsheet Controllers

TAG	Description	Set-Point
LeanSolvent_FC	Lean solvent to absorber flow controller	5674.60 kg/h
FlueGas_FC	Flue gas to absorber flow controller	2248.37 kg/h
COND_LC	Flue gas condenser level controller	5.33 m
ABS_DrumLC	Absorber sump level controller	1.00 m
WASHTOW_PC	Absorber wash tower pressure controller	1.05 bar
WASHTOW_LC	Absorber wash tower level controller	1.83 m
BUFFER_LC	Buffer tank level controller	2.25 m
REGEN_CondPC	Regenerator condenser level controller	1.80 bar
REGEN_DrumLC	Regenerator top level controller	0.64 m
REGEN_SumpLC	Regenerator sump level controller	1.70 m
LeanTC	Lean solvent from heat exchanger temperature control	50.50°C
SteamFC	Steam to regenerator reboiler flow controller	500 kg/h
LeanColdTC	Lean solvent from cooler temperature control	41.80°C
Tank_PC	Storage tank pressure controller	1.00 bar

3.0 TUTORIAL

3.1 Reaching an Initial Steady-State

This example shows how to drive the process model from one steady-state to another. The lean solvent flowrate to the absorber is used as an example. Similar approach can be taken for perturbing other controlled variables.

1. Open the “CCSI_MEAModel_dynamic.dynf” file.
2. In the “Process Flowsheet Window,” double-click the controller “LeanSolvent_FC” to open the controller configuration window.

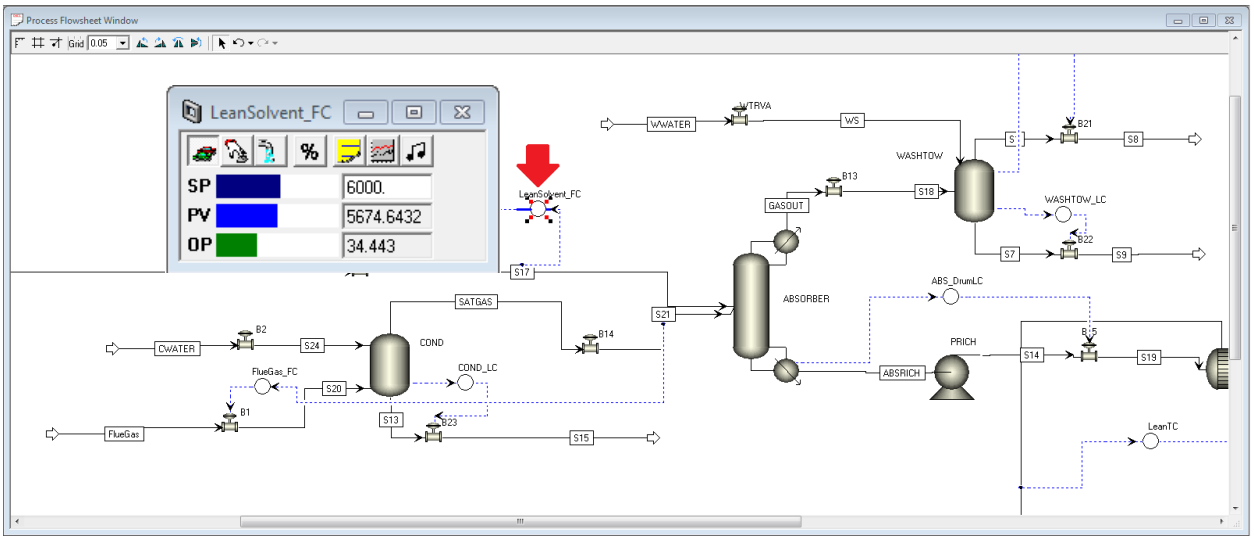

Figure 2: “LeanSolvent_FC” configuration window.

3. On the configuration window:
    a. Make sure the controller is in “auto-mode” as illustrated in Figure 40.
    b. Set “SP” to be “6000 kg/h.”

4. In the “Contents of Simulation” pane, located in the left side of the window, double-click “Flowsheet,” a new list of local files and options displays. Double-click the “Lean_Solvent” Form. Figure 41 illustrates this step.

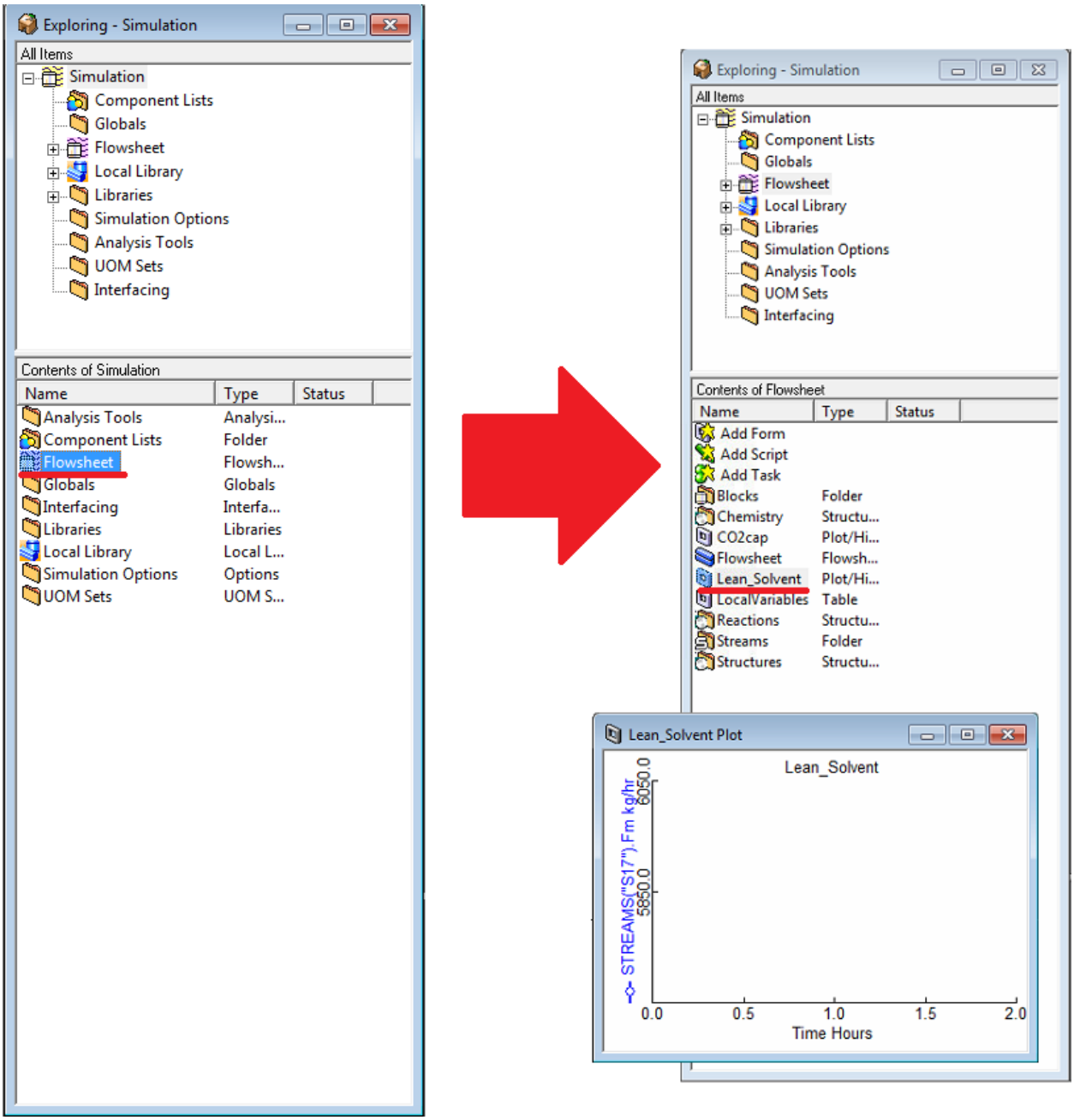

Figure 3: Opening a form.

5. Double-click the “x-axis” of the plot to open a configuration window that shows the axis properties. The default value for the time window is 2 hours, change it to “8.”

6. On the toolbar, click “Run Options,” as highlighted in red in Figure 42. Under “Simulation control,” change the “Pause at” value to “8” hours, which should be adequate to reach a new steady-state. This feature is very useful to introduce new step changes in the model, or to simply end the simulation at a given time.

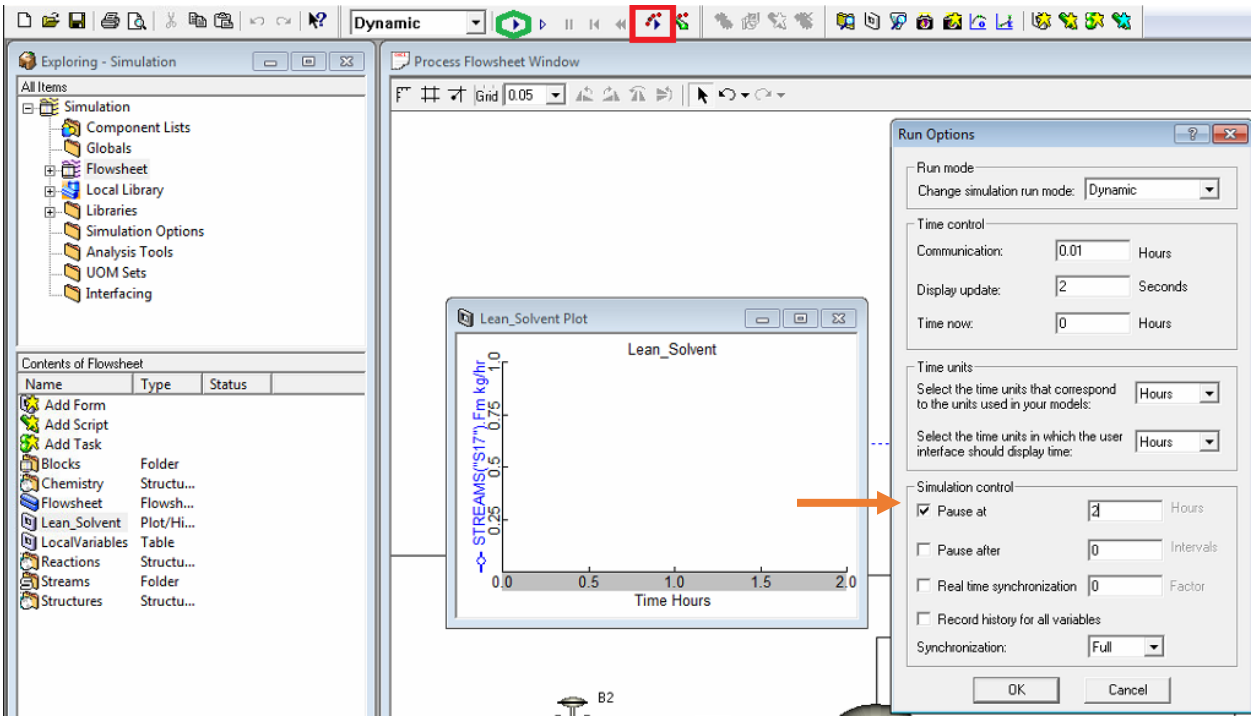

Figure 4: Run options.

7. Run the simulation by clicking “Play” as highlighted in green in Figure 43. The “Lean_Solvent” window records the behavior of the variable during the simulation. A plot similar to Figure 44 is expected. Figure 45 is a magnified version of the plot in Figure 44 showing the initial dynamics of the process.

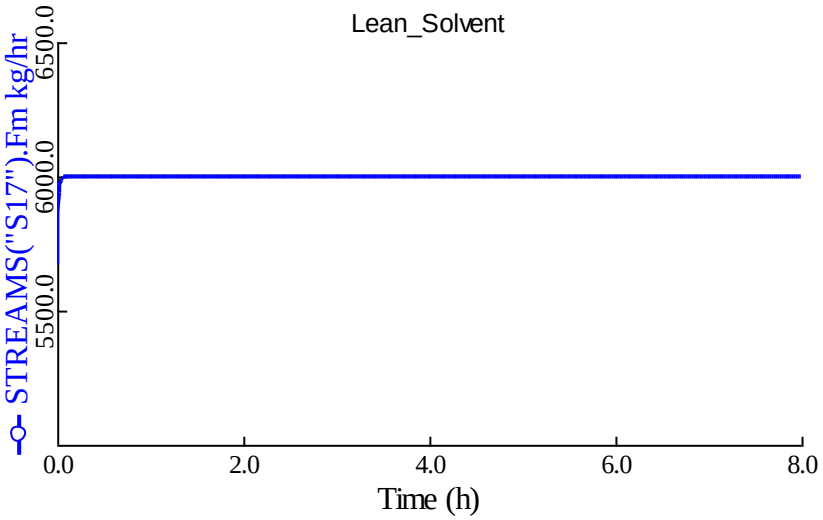

Figure 5: Lean solvent flowrate behavior during step change to a new steady-state.

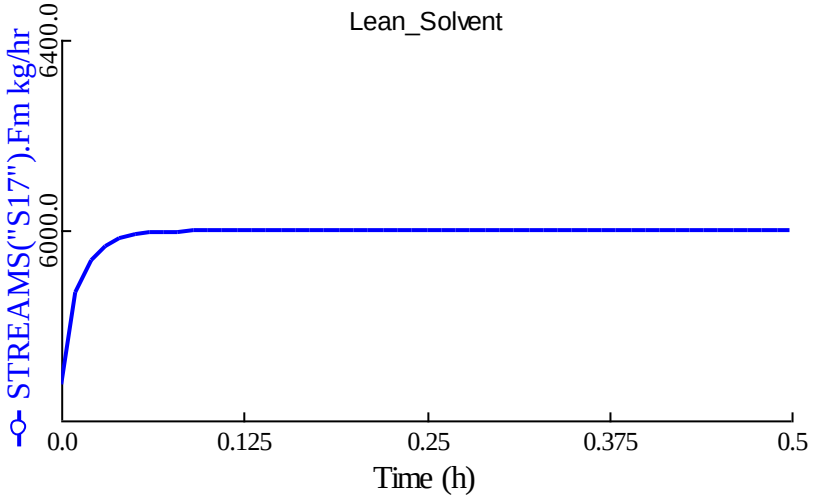

Figure 6: Lean solvent flowrate behavior during step change to a new steady-state (0.5 h).

3.2 CO_2 Capture Dynamic Response Simulation

After a desired steady-state is reached, a number of step changes can be introduced to the system. In the beginning of this simulation, the lean solvent flowrate is at 5674 kg/h, which is the default lean amine flowrate when the file is opened.

1. Open the "CCSI_MEAModel_dynamic.dynf" file.
2. In the "Contents of Simulation" pane, located in the left side of the window, double-click "Flowsheet," a new list of local files and options displays. Double-click "Lean_Solvent" Form and change the x-axis time window to "2" hours.
3. Repeat Step 2 for the "CO_2 capture" Form.
4. On the toolbar, click "Run Options," as highlighted in red in Figure 42. Under "Simulation control," change the "Pause at" value to "0.50" hours.
5. Run the simulation until it is paused.
6. In the "Process Flowsheet Window," double-click the controller "LeanSolvent_FC" to open the controller configuration window and then set "SP" to "6000."
7. On the toolbar, click "Run Options," as highlighted in red in Figure 42. Under "Simulation control," change the "Pause at" value to "1.0" hours.
8. Run the simulation until it is paused.
9. In the "Process Flowsheet Window," double-click the controller "LeanSolvent_FC" to open the controller configuration window and then set "SP" to "5674."
10. On the toolbar, click "Run Options," as highlighted in red in Figure 42. Under "Simulation control," change the "Pause at" value to "1.5" hours.
11. Run the simulation until it is paused. Results similar to Figures 45 and 46 are expected.

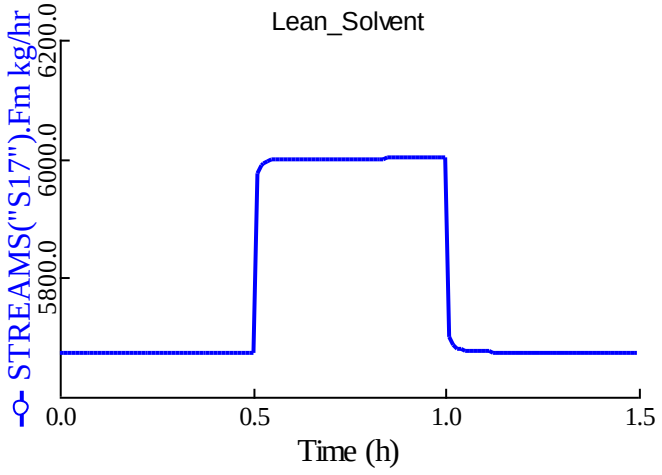

Figure 7: Lean solvent flowrate into absorber.

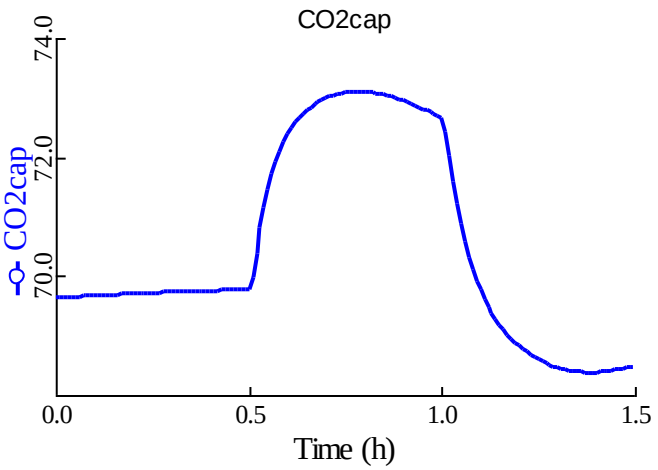

Figure 8: CO_2 capture percentage.

4.0 REFERENCE

1. Zhang, Qiang; Turton, Richard; Bhattacharyya, Debangsu. Modeling and model predictive control of a MEA-based post-combustion CO_2 capture process. Review Submitted, *Industrial & Engineering Chemistry* Research, 2015.

2. Morgan, J.C.; Bhattacharyya, D.; Tong, C.; Miller, D.C., Uncertainty Quantification of Property Models: Methodology and its Application to CO_2-Loaded Aqueous MEA Solutions. *AIChE Journal* 2015, 61, 1822-1839.

3. Plaza, J.M. Modeling of Carbon Dioxide Absorption Using Aqueous Monoethanolamine, Piperazine, and Promoted Potassium Carbonate. PhD Thesis, The University of Texas at Austin, 2012.

4. Mathias, P.M.; Gilmartin, J.P., Quantitative Evaluation of the Effect of Uncertainty in Property Models on the Simulated Performance of Solvent-Based CO_2 Capture. *Energy Procedia* 2014, 63, 1171-1185.