**Introduction to ChemCad for CME 415: Separations**

ChemCad is a steady state chemical process simulator. A process simulator is a specialized calculator which enables you to sequence the equations that “model” unit operations in a useful way, specify enough variables to reduce the degrees of freedom to zero, and then simultaneously solve a large number of interrelated equations for the unknown variables.

A steady state simulator solves for the unknowns assuming sufficient time has passed so that system variables no longer vary with time. In many cases, this results in algebraic equations instead of differential equations which must be solved. Other examples of steady state simulators include HySim and ASPEN. Unsteady state simulators are required to solve often thousands of simultaneous of partial differential equations and require a higher degree of sophistication. The best example of an unsteady state simulator is Aspen SPEEDUP.

The instructions provided here are designed to instruct in use of ChemCad by Chemstations, Inc. The principles of simulation design may be applied to other simulation packages. The example used to illustrate use of ChemCad is focused on the issues that may arise when using ChemCad to simulate separations processes.

Additional reference material can be found in the ChemCad Version 5.0 User Guide and Tutorial (available from Dr. Silverstein), in the examples found in the CC5DATA\Examples directory on the machine with ChemCad installed, online at [http://www.chemstations.net](http://www.chemstations.net), and in the extensive (but not well organized or indexed) help system accessible from within ChemCad.
Steps to a Simulation

- Start a new job
- Select Engineering Units
- Create Flowsheet
- Select Components
- Select Thermodynamic Options
- Define Feed Streams
- Input Equipment Parameters
- Run the Simulation
- Review and Output the Results
- VALIDATE THE RESULTS

The remainder of this tutorial will explore the above steps in terms of a problem from your textbook.
Start a New Job

File/New

Give the job a name. A separate directory is created for you with the name of the job. ChemCad uses numerous files to track the data and output for a job, all of which are stored in a single directory. Consequently, you will need to submit all of those files when doing homework (or asking questions about) using ChemCad so that your modeling efforts can be accurately reviewed.

Select Engineering Units

Format/Engineering Units

You need to look at the units you have data in and the units you want your output in while planning your simulation. ChemCad does allow changing some units from within individual unit operations, but you should select your default units here. Note you can choose SI, CGS, English, or define your own subset of useful units. Save your self-defined unit combinations if you think they will come in handy again.

Create Flowsheet

You need to be in Flowsheet mode in order to create unit operations, streams, feeds, or products. The current mode is indicated in the status bar at the bottom of the ChemCad window. You can switch modes from the menu (if in Flowsheet mode, Run Simulation is an option; if in Run mode, Edit Flowsheet is an option).

A flowsheet is typically designed using the palette of icons. The first row of icons represent fundamental operations and graphical shapes. The arrow cursor allows you to select an object on the flowsheet. The overlapping squares allow you to rotate an object. The remaining icons on the row allow you to create geometric shapes to ornament and enhance your flowsheet. These objects will not play a role in your simulation. The next icon allows you to place text on the flow sheet.

The right angle line segments with blue and red tips allows you to connect streams between unit operations. All unit operations in the system must be connected to feed and
product blocks either directly or through other unit operations in the simulation. The blue tips indicate inlet connectivity and red tips indicate outlet connectivity.

The remainder of the icons represent unit operations. As your run your mouse cursor over the various icons, you will see a description of the icon in the status bar. For some unit operations, you will be informed as part of the description that there are other icons that may be accessed by right clicking on the “parent” icon. These icons will vary by picture or by number or location of inlets and outlets, but the fundamental operation is the same.

The unit operations are arranged alphabetically by name. Detailed information is available about each unit operation by using the online help system. Some operations you may be interested in for this course include: batch column; component separator; crystallizer; extractor; flash; LLV flash; SCDS Column; Shortcut Column; Tower; Tower Plus.

In addition to the unit operations, a feed and product arrow are included in the icon tray. A feed is a unit operation containing a single outlet stream; a product contains one inlet stream. All simulations must begin with a feed and end with a product block.

After placing your unit operations you should use the stream tool to connect inlets and outlets. ChemCad lets you know when your cursor is in the right place to connect a stream by telling you if a node is an inlet or an outlet. To stop drawing streams, click the right mouse button and make the appropriate selection.

Note that ChemCad has assigned a number to each unit operation and stream. This is convenient for certain applications, but when drawing a flowsheet to be presented to others, it is helpful to give meaningful names to operations and streams. You may right click on a block and choose Edit Name to give a more meaningful (but brief) name to the object. Use the text tool when appropriate to supply further information. Remember that in addition to setting up a simulation, you are also using your flowsheet to communicate information to the people who will review your simulation.

**Select Components**

At this point we need to switch to simulation mode by selecting Run Simulation from the menu. In Simulation mode, you must now tell ChemCad which chemicals will appear at any point in the simulation. This includes species present in any phase: air, water, solids, etc.
Remember that aqueous solutions include water! If oxygen is involved explicitly with any operations, you are better off choosing oxygen and nitrogen separately rather than using air.

ThermoPhysical/Component List

The search for box uses a “substring” search, so after typing the name of your compound, your desired chemical may not be selected. Use the “next” button to move down the list of species containing that substring. You may also use the empirical chemical formula of a species in your search. After moving all the required chemicals onto the selected components list using the “add” button (or double-clicking on the species in the databank list), click OK.

Select Thermodynamic Options

You have to tell ChemCad what thermodynamic model is best for predicting the physical properties of the species involved in your simulation. These properties are in turn used for everything from predicting K-values to melting points of mixtures. You have two basic choices for how to choose the model. You can give ChemCad some basic information such as the temperature and pressure range of interest and let it recommend a model, or you can choose a model. In general, you should determine a suitable model on your own based on your training, research, and experience.

ThermoPhysical/K-values

Multiple options are available including UNIFAC, SRK, Peng-Robinson, and others. You can specify your own data in appropriate forms. The bottom line is you need to find a model that works for your system. Note that at this point you are only defining the default choice of the thermodynamic model. Many operations allow you to specify a different model for conditions specific to that block.

You also have options for models for determining enthalpies, fluid transport properties, and specifying binary interaction parameters. In most cases, unless you know better, you are mostly likely better off using the default selections for these properties.

Define Feed Streams

You need to specify your feed stream(s) for any simulation. Note that you may not overspecify a stream. Your choice of which variables to specify is important: If you specify a
pressure and a temperature, ChemCad performs a flash calculation to determine the vapor fraction of the mixture. If you specify the vapor fraction as 1, a dew point calculation is performed (temperature if pressure specified, pressure if temperature specified). A vapor fraction specified as zero causes a bubble point calculation to be performed. This is a quick way to make some basic calculations involving flashes. It also gives you an easy way of checking if your chosen thermodynamic model has a hope of working for your system.

**Input Equipment Parameters**

Each unit operation has a collection of parameters which may be specified for your simulation. Some are required, others are optional. While the help files will indicate what each parameter is, you still need to understand what the relevance of each parameter is to the calculation you will perform. ChemCad will try to catch errors before accepting entries, but will not catch all errors you make.

**Run the Simulation**

Before running the simulation ChemCad checks again to see if there are any obvious errors in your simulation specifications. If there are no errors or warnings, or if you choose to proceed anyway, ChemCad will finish the simulation in a few moments. Don’t let me get started on how long these simulations used to take.

**Review and Output the Results**

ChemCad can present results in several different ways. It can give you stream data in tabular form. It can give you properties. It will due special plots like T-x-y and residue curves. It will do column profiles. All of these options are present under the Plot and Results menu items. You can also prepare more formal process flow diagrams (PFD) using the Output menu items. Some equipment sizing can be performed using the Sizing option. Other utilities including a unit specific calculator can be found under Tools.

Most of the time you will want to take the WordPad files with tabular data and import those files into Excel or Polymath. You may also want to use the T-x-y and x-y diagrams as
prepared in ChemCad, though you have the option to export the data to an Excel compatible format.

VALIDATE THE MODEL

ChemCad has no capability to exercise judgment. It only takes the data you provide and makes calculations. It is up to you to determine if the model is reasonable or not. You will learn much more about validating models in CME 420. For now, you should focus on validating the thermodynamic model choice, and comparing results to experimental data and hand calculations. This is a critical step in the modeling process and may not be omitted.