# CAD/Chem

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Formulation involves mapping from product ingredients and processing conditions to product properties, a problem faced by a wide range of companies. CAD/Chem is an intelligent software application for designing such formulations. Any problem that can be couched as one of formulation is a potential target for CAD/Chem, including plastics, metals, pharmaceuticals, industrial chemicals, and food goods.

The traditional approach to formulation involves experimental trials followed by statistical analysis; the resulting model is used to optimize a set of ingredients. This product development process can require an enormous amount of experimental work and difficult statistical analysis, both of which can be costly. CAD/Chem tries to ease this burden by applying intelligent technology, primarily neural networks, in a window-based software environment to the modeling and optimization of product formulations.

## Installation

Although we had some problems, installation of the software was relatively seamless. Some of the problems we had were due to security restrictions placed on CAD/Chem by its developers. The software came on the appropriate media (in this case, a 1/4-inch cartridge tape). First, we transferred files to a target machine in our distributed, networked environment, and then executed installation utilities. However, the software under a single-user license can only be run on the workstation that it is authorized for, and *must* reside on the local disk. That meant we had to find a stand-alone workstation with enough disk space and a connected tape drive. Furthermore, the software cannot be run on the local workstation and displayed on another workstation's display using the standard X and Open Windows methods. In all, we had to call the company twice regarding the software authorization key, and go through two installation procedures. CAD/Chem is available under multiuser licensing, but still, I was a little surprised at the restrictiveness of the single-user license.

To evaluate CAD/Chem, I used a Sparcstation 1 with a 20-MHz Sparc processor. The workstation was equipped with 8 Mbytes of main memory (the minimum for CAD/Chem) and 24 Mbytes of swap space. The display was a 19-inch monochrome monitor with a simple frame buffer video card. The workstation was running Sun-OS 4.1.2, and Sun's Open Windows version 3 windowing system. CAD/Chem also runs on several other workstation platforms, including Hewlett-Packard, IBM, and DEC.

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## Operation modes

CAD/Chem runs in three modes: a consult mode for manipulating the product model, a data-processing mode for loading and repairing data and resolving data conflicts, and a training mode for creating the model. The package comes with two examples that can be used to explore these modes. To prepare this review, I used both the bread formulation example (which is the basis of the tutorial) and the polymer additive example.

**Consult mode.** CAD/Chem is most often used for consulting; model formulation is usually done only once (unless new data is available). You begin in the consult mode with the Open Task window, which displays a list of task names; you point to the desired task and open it. This mode also offers the Home window, which is the base of operations in all modes and is always active, and a Message window for error and operation completion notices. Much of the CAD/Chem interface is point-and-click and, for the most part, well designed, with command buttons, menu buttons, and scrolling lists. (Later I'll discuss the few interface problems I encountered.)

Once you've opened a task by clicking on its name and the Apply button, the Consult Task window appears. This becomes the base of operations for all consult mode activities: using the formulation model to find matches to the current ingredient or property trials (Best Match), determining the impact of ingredient changes (Estimate), and optimizing ingredients for specific goals (Optimize). The task displayed by the Consult Task window has already been trained (the training mode will be discussed later). The Consult Task window is dominated by two scrolling lists, one for ingredients on the left and the other for properties on the right. Each list contains columns for the name and units, as well as Given and Found columns. The Given column lets you type in values (one of the few times it is necessary to use the keyboard), and the Found column displays values based on some operation (for example, Estimate). In the case of the bread task, there are 10 ingredients, including flour, water, and bake time, and 13 properties, including moistness, weight, and sweetness. Processing conditions such as bake time are considered ingredients.

Above and below these two scroll lists are various command and menu buttons for consult mode operations. CAD/Chem's use of Open Windows' push-pin feature lets users continuously display and access the most commonly used menus. In window environments where the push-pin feature is not available, the interface is more cumbersome. I tried both menu access approaches (with and without the push-pin feature); for sessions where access to the Ingredients and Properties menus dominated, the push-pin feature was almost indispensable. In most sessions involving the consult mode, these

are the most accessed menus. The documentation suggests pinning these menus so they are immediately accessible.

The Best Match option allows the recall of experimental trials (ingredient or property lists) based on complete or partial information. Matching is based on a least mean square closeness measure. After you type the match information into the appropriate display and choose either the Best Ingredient Match or Best Property Match command button, the system finds the matched values and displays them in the Found column. This operation ignores blank entries in the Given column, but tries to match zero entries. The Best Match option is a good starting point for exploring how changes in ingredient amounts affect properties. The recall processing of Best Match is nearly instantaneous.

The Estimate option is used to explore the effect of ingredient changes on product properties. A trained task contains a model of the relationships between ingredients and properties. By supplying a complete set of ingredients, the formulation model can estimate the values of the properties of the new formulation. In this way, the user can perform "what-if" scenarios exploring the effect of changes in the ingredients. In the bread task, you can increase the amount of salt or decrease the amount of water, and then view the impact on the bread's properties, such as crust thickness, tenderness, and texture. You type in the ingredients (or edit an existing list) and then click on the Estimate Properties command button. Like the Best Match operation, Estimate is very fast. The property values for the new formulation are displayed in the Found column of the Properties display list, just as they are for the Best Match operation. An option in both the Ingredients and Properties menus is to move the values in the Found column to the Given column. This is a useful way to store property values before performing the Estimate operation and provides a side-by-side comparison of the effect of ingredient changes.

Using Optimize, you can determine the set of ingredients needed for a particular set of properties. Unlike the relatively unstructured process of using the Estimate operation in successive "what-if" scenarios, the Optimize operation involves a systematic search using the formulation model to determine the appropriate ingredients. Optimize is CAD/Chem's most powerful feature and requires the most care in use. There are a host of parameters that you can set to guide the optimization process toward a satisfactory answer. These include ingredient costs, ingredient constraints, property weights, and property desirability functions. The window interface displays for setting these parameters are accessible through the Ingredient and Properties menus in the Consult Task window.

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Once the parameter values are acceptable, you click on the Optimize Ingredient command button, and the Optimization window appears. This is the base of command for the Optimize option: From this window, you start the optimization process, view its progress as ingredient, property, and property desirability values change, and track the overall process in terms of total cost, total desirability, and a utility index. The Optimization window also gives you access to optimization tuning parameters. To begin optimization, you click the Optimize command button. Unlike the Best Match and Estimate operations, which are performed in seconds, Optimize takes several minutes. This operation should not be applied casually; you must first define the problem carefully in terms of ingredient costs and constraints, property weights, and desirability functions.

Another feature of the consult mode is its graphing capabilities, which are quite good. CAD/Chem produces 3D plots of the formulation model. Two ingredients (the independent variables) are plotted on the $x$ and $y$ axes, and the selected property or desirability function (the dependent variable) is plotted on the $z$ axis. The interface for graphing is simple: You click on the Graph command button in the Consult Task window. The Graph window appears, allowing you to set the $x$, $y$, $z$ quantities, the $x$ and $y$ minimum and maximum, as well as the number of tick marks. You then click on the Plot command button, and a Grid window appears displaying the 3D plot. Generating the Grid window took a little more than 20 seconds. Once the Grid window is displayed, the 3D plot can be manipulated in near real-time using the Rotate and Tilt slider controls. CAD/Chem allows multiple plot displays; in my testing, four Grid windows were displayed at once on the workstation display, with no degradation in generation time or manipulatability. It is tempting to spin the plotted surface in all possible directions, but it can be difficult to return to a specific view if you forget to note the original tilt and rotation. In orthogonal views of the surface, the min/max labels can appear on top of each other, making them difficult to read. The 3D surface itself can be viewed as a wire frame, a solid, or a color solid with shading. For this review, I explored only the wire frame and solid features. The solid and color options appeared identical on my monochrome display.

Cad/Chem can generate reports for documenting the values used in the consult mode, such as the cost of ingredients, ingredient constraints, and property desirability functions.

I had a few problems with the consult mode. There was a discrepancy between the documentation and the working of CAD/Chem's Ingredient Costs window, which lets you type in values for each ingredient's cost. In the documentation, the value of *eggs* is 125.25, and the value of *bake-temperature* is 355.00, but the interface rejected these values when I entered them. The error message reported that the values had to be between 0 and 100. This presents an interesting conflict for users, since the formulation might include small amounts of very expensive ingredients. If users are expected somehow to normalize all costs to a scale of 0 to 100, this means a lot of extra work and can present difficulties as ingredient prices change. Additionally, only the relative costs of ingredients would be displayed, not their actual costs.

The Ingredient Constraints window interface could be improved in three ways. The system uses the symbols i1, i2, and so forth to represent the ingredients in the equations. Thus, to interpret an equation you must remember, for example, that i5 is Milk. This information is available as a scroll list in the display, but if there are a lot of ingredients, you might have to refer often to this list. The software knows the ingredients' names, so why not use them to construct and display the constraint equations? The equation Flour > 0 is superior to i1 > 0; for the user, the same input effort would be required if the ingredient names were available using point and click. The Ingredient Constraints window uses a calculator keypad for inputting the relational operators (<, >, and so on) and the numeric constants that the ingredients are compared to. This is nice if you don't like to type, but the display should give skilled typists the complete use of the keyboard to enter equations. The calculator keypad has a nice look, but its speed of entry is not superior to a keyboard. Lastly, the software should identify conflicting constraints and alert the user. Currently, the user must make sure that the constraint equations are consistent.

**Data-processing mode.** To move beyond consulting and build your own formulation model, you use the product's loading, analysis, and training modes. CAD/Chem accepts formulation data in simple ASCII format, which can be followed easily using a standard word processor or created from a spreadsheet or database. To load a data file, you work from the Home window and choose Load Data from the Mode menu. The Load Data window appears, and looks very similar to the Open Task window. However, you must supply a file filter (*.dat) when changing from one directory to another with the CD command button. You click on the data file to be loaded, for example bread.dat, and then on the Apply command button. A second Load Data window appears; you use this to select which elements in the data are ingredients and which are properties, and enter the units for these items. The Load Data window is also the base of operations for renaming tasks and for editing, repairing, and filtering data. You can repair incomplete data sets easily using either the repair function or the data point clustering feature (based on unsupervised learning). The software also examines the data set for conflicting patterns and lets you remove or edit these patterns. Conflicting patterns (when two or more data sets are identical or nearly identical) should be removed before training begins.

**Training mode.** CAD/Chem's training mode is quite extensive and allows you to be involved in the training process as much as you want. If you are very "hands-off" about constructing the neural-network model, the autotrain feature is handy; for more involved users, the interactive train feature lets you manipulate the training process extensively.

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I tested autotrain, described in the documentation tutorial. From the Home window, you select the Open button from the Mode menu. The Open Task window appears, and you click on the task to be opened; if the task has not been trained, the Train Task window automatically appears, and you click on the Train command button. This window is the base of training operations. It displays a number of statistics, including the learning rate, momentum, and sigmoidal slope, as well as the number of iterations and status of the training process. For the examples provided, the training was fairly fast and very easy to accomplish. Once trained, a task can be used in the consult mode and operations such as Optimize can be performed.

In the interactive-train feature (not tested for this review), the documentation reports a host of features, including user-determined correlation coefficients, variation of training parameters and network structure, and step-by-step interaction with the training task.

**Promotional material**

AI Ware offers an 18-page technical document on CAD/Chem as well as an article preprint from *Scientific Computing and Automation* that describes the use of CAD/Chem in formulation work. The technical document discusses only the consult mode in detail; it provides just a couple of pages on loading data and the possible data analysis options. There are no hard details on developing a formulation model using the various neural-net training options. AI Ware also has an advertising video that demonstrates CAD/Chem's consult mode but does not discuss training, loading, or analyzing data. AI Ware can provide a list of customers and contacts in both industry and research, who span a variety of fields, including chemicals, materials, and processing.

All in all, CAD/Chem is an interesting product and one you might consider if faced with formulation problems. Test the software using representative example data from your target application to ensure that it can meet the needs and scale of your application. This is the best way to determine if CAD/Chem can meet the challenges of your own formulation tasks.

***Reader service number 21***

*CAD/Chem from AI Ware, 11000 Cedar Avenue, Cleveland, Ohio 44106; (216) 421-2380. Available for IBM RS/6000, Hewlett-Packard, Sun, and DEC VMS and Alpha workstations. Prices are based on the number of concurrent users, and range from $9,000 for a single-seat license to $30,000 for a fully networked, single-site system. The package comes with user documentation, installation instructions, and 90-day free maintenance. Extended maintenance contracts are available for hotline phone support and all documentation and software updates. Additional user training and custom enhancements are available. The company plans to release a PC version in November.*

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