

Computer-Aided Thermodynamic Tables 3 -- CATT3

This is the final installment in our series on CATT3. If you haven't read Part I, make sure you do so first here. In this section of our series on Computer-Aided Thermodynamic Tables 3, we will explore how to optimize parameters for a desired system output. When maximizing or minimizing specific outputs, the user must specify what variables are specifically relevant to that output and define what variables are not relevant. The difference between these two must be accounted for within the optimization routine itself, which can have some interesting consequences depending upon system design. We will take a look at how to optimize the retention time of a liquid, which is an important variable for certain types of filtration processes. We will use the following procedure to do the optimization: (1) Define variables relevant to liquid retention time. (2) Define linear relations between each relevant variable. (3) Define non-linear relations between each relevant variable. If you are performing analyses involving viral immunity, you may wish to include viral load as part of the liquid retention time, however if this is done it must be done explicitly within the model itself within the algorithm corresponding to this objective function. (4) Define the final objective function. Here is a good example of how good model creation can save time and money:

Let us try to predict the amount of marinade that is required to properly coat the surface area of a cut of beef without leaving any excess marinade on it. We will use CATT3 for this analysis. Using CATT3, we first define what variables we consider relevant: The first step in creating a model is defining which variables are relevant and which variables are not relevant. In this step, we define the relevant variables to be: formula_36, formula_37, and formula_38. The marinade formulation of interest is given by: formula_39 The not-relevant variables are the solubility of the marinade in water and concentration. Then we define a basic model of this linear system of equations:

Using CATT3, we can then use a thermodynamic approach to optimize for a specific output variable, in this case the amount of marinade required to properly coat a cut of beef without any excess on its surface area. In this objective function, TDS is the system temperature which is calculated from the bath temperature and bath volume. Tmax is the maximum surface area that a cut of beef can have before it begins to dry out. For this example, if we use a model based on this objective function, we will have a model with 1 solution. The first step in creating a model is defining which variables are relevant and which variables are not relevant. In this step, we define the variables relevant to the marinade formulation as: formula_35, formula_37, and formula_38.

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