

OLI Tips #8

Calculating heat capacity in OLI/ESP

The heat capacity of a solution can be defined by the following equation:

$$C_p = \left. \frac{dH}{dT} \right|_p$$

The OLI Software automatically calculates this as part of its numerical equation solving. The enthalpy of the solution is calculated and its temperature derivative determined. This enthalpy is the total enthalpy of the solution including any vapor, aqueous, liquid and solid components.

There are two methods of determining the heat capacity.

Method 1: Numerical method

In this method, the user creates a stream with the temperature, pressure and composition. An isothermal calculation is performed. This can be done using a process block such as a mixer or using the ScratchPad feature. The enthalpy of the total stream is recorded.

A second calculation is performed at a slightly different temperature. Usually we perturb the temperature between 0.1 °C and 1.0 °C. Any larger perturbations introduce some numerical noise to the calculation. The composition and pressure remain constant and a new enthalpy value is recorded. The change in enthalpy is divided by the change in temperature. This is approximately the heat capacity.

$$C_p \approx \frac{H_{T+\Delta T} - H_T}{\Delta T}$$

Method 2: Direct calculation

The second method is more involved. The user must modify the chemistry model (the MOD file) directly. The following section should be added to the chemistry model:

```
EQUATIONS  
DEFINE CP=USER20(54)
```

This adds a new variable to the model and calls a FORTRAN subroutine which evaluated the heat capacity.

The chemistry model generation is then completed normally.

To obtain the heat capacity in the process, the user must first select a ***Calc Aid*** option known as ***Set Trace = ON***. This will produce a supplementary file with the file extension of OUE. In this file will be all the calculations performed for each stream and unit in the process. The Heat capacity will be reported. The Heat Capacity is for the entire stream, all phases considered.