The EOS calculations used here involve the following components:

- Commercial EOS software to supply fluid thermodynamic and volumetric properties. SNL modified this software to accommodate modeling the Macondo reservoir crude oil.
- SNL created computer routines to do the following:
  - Calculate pressure drop in a crude oil mixture for various flow path geometries, including the well itself and various kill- or choke-line configurations.
  - Flash crude oil into liquid and gas phases as required and based on the pressure drops calculated above.

Despite the fact that the above two activities interrelate and often require iteration, each of these issues is discussed separately below.

The SNL Team started with a commercially available Microsoft Excel™ add-in EOS, the Moongate equation of state. The SNL Team then modified this product's list of available components to include heavy crude pseudo components (the 15th and 16th entries in Table C.1). This add-in provides liquid and vapor thermodynamic and volumetric properties for mixtures of compounds as Microsoft Excel spreadsheet function calls. The user is responsible for combining these function calls into algorithms.

The original software package includes both the Peng-Robinson and the Lee-Kesler Plocker EOS models (References C.1-C.3). The package uses the Peng-Robinson EOS to provide components' fugacity coefficients used in a flash calculation. The software package uses Peng-Robinson, because the Lee-Kesler Plocker EOS fugacity coefficients can be unstable near the critical point. All other volumetric and thermodynamic calculations are performed using the Lee-Kesler Plocker EOS. This EOS is more accurate away from the critical point, particularly for liquids, than is the Peng correlation.

Both equations of state are curve fits to Pitzer's corresponding states model. The Peng-Robinson uses a cubic polynomial. The Lee-Kesler Plocker incorporates a more complex combination of two sixth-order polynomials, each combined with exponential terms.

Nonideal thermodynamic properties, such as enthalpy, fugacity, or entropy, are estimated using standard departure-function methods.

In the two-phase region, the calculation is complicated by the partitioning of the various components between the gas and liquid phases. In equilibrium, the materials in the vessel sort themselves out, such that each component contributes the same energy to total pressure in the vapor phase as in the liquid phase. If the vapor and liquid mixtures were ideal, each component's partial pressure in the two phases would be equal. Crude oil mixtures are far from ideal, so each component's fugacity takes the place of partial pressure. In other words, at equilibrium,

$$f_i^V = f_i^L \qquad \text{C.1}$$