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## **Errata and clarifications for Thermodynamic Standard specification 1.0**

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## SUMMARY

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The errata and clarifications have been discussed and developed by the CO-LaN Special Interest Group dedicated to CAPE-OPEN “Thermodynamic and Physical Properties” interfaces. Although version 1.0 is part of the current CAPE-OPEN standards, new developments should use the version 1.1 specification instead.

### 1.1 Clarifications:

#### 1.1.1 Naming convention of liquid phase

The naming convention of phases status: “It is advised to use the name “Liquid” for the first liquid phase, and the name “Solid” for the first solid phase. In the above table, X is a place holder for any name, so “LiquidX” could be for example “LiquidWater”, “Liquid2””. A clarification is justified here: unit operations may assume that a phase called "Liquid" is present and issue a calculation for a property of such a phase, i.e. "Density" of phase "Liquid". As a unit operation has no means of querying the total list of phases, it is not feasible for a unit operation to find any existing liquid phase in case the phase "Liquid" is not defined. Hence, in case liquid phases are present, at least one of them should be called "Liquid".

#### 1.1.2 Errors during CalcProp

Section 5.2.2 states that in case of multiple property calculations, no property should be set on the Material Object if any of the property calculations fails. This also holds for a single property calculation: in case CalcProp returns an error (of any kind), the content of the Material Object should not be changed.

#### 1.1.3 heatOfVaporization

The definition of the non-constant property heatOfVaporization is ambiguous. It could have the meaning of the heat of vaporization for a pure compound on the saturation line, or it could be the difference of the enthalpy of the vapor and liquid phases at given conditions (T, P, composition). Other definitions are conceivable. Due to the fact that existing software implementations may serve or consume a different interpretation of this property, it is advised not to use this property, and use enthalpy differences instead.

Version 1.1 gives a clear definition of this property, which is a temperature dependent property for pure compounds and defined at the saturation line. Applications are advised to move to version 1.1 in case the use of property heatOfVaporization is required or desired.

#### 1.1.4 ResolvePropertyPackage

The Thermo System expects the name of a property package that is defined on the system to be passed to ResolvePropertyPackage. These names are returned by GetPropertyPackages.

In case Property Packages can be persisted, the situation is somewhat more complex. The Property Package may have been created at a different computer, or the list of available property packages may have changed since the property package was first created. In this case, ResolvePropertyPackage returns an uninitialized

Property Package, that keeps track of the name that was specified. In case the Property Package had been persisted, a call to Load will follow, and the Property Package receives its configuration data. In case Load is not called, the Property Package still need to receive its configuration data during Initialize. An invalid name passed to ResolvePropertyPackage leads to an error in Initialize.

So passing an invalid name to ResolvePropertyPackage may lead to an error immediately for Thermo Systems of which the Property Packages cannot be persisted, or may lead to an error during Initialize if the Property Package if persistence is supported but the Property Package was not loaded from persistence.

In either case, the PME has the responsibility to expose to the user any textual error message provided by the Property Package.

### **1.1.5 Notes on recommended error codes**

Section 5.8 states that the version 1.0 thermodynamic standard specification does not provide recommended error codes for common error scenarios. Still each method should, when failing, return error codes according to the Error Common Interface specification and its client should query the error handling interfaces for error details so that the end-user may be properly informed of the error conditions.

## **1.2 Errata**

### **1.2.1 GetPropList**

The descriptions of GetPropList for ICapeThermoMaterialObject and ICapeThermoPropertyPackage should refer to the non-constant property list in table 3.10.3; constant properties in table 3.10.1 should not appear in the list returned by GetPropList.

### **1.2.2 Initialization and termination**

Section 5.10 discusses initialization and termination activities on Thermo Systems and Property Packages. The second paragraph of this section starts with "A Property Package that is created from a Thermo System is, in accordance with the definition of PMC Primary Objects and PMC secondary objects *in the also* a top-level CAPE-OPEN object". It should say "A Property Package created from a Thermo System is, in accordance with the definition of PMC Primary Objects and PMC Secondary Objects, also a PMC Primary Object."