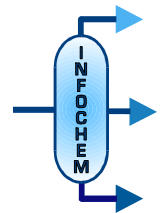


# Beyond VLE – a Thermo 1.1 Property Package

Infochem Computer Services Ltd

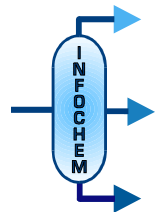
Richard Szczepanski

CO-LaN Cannes meeting  
March 2006



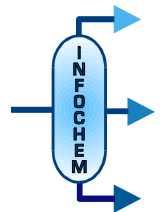
# Outline

- Objectives of Thermo 1.1 specification
- Phases in Thermo 1.1
- Experience of implementing a 1.1 Property package
- Demonstration
- Conclusions



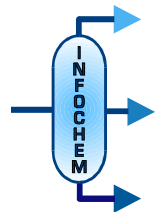
# Objectives of 1.1 Thermo spec

- Make the specification a useful working document for developers
  - Clarity
  - Explain the purpose of each method
  - Indicate how it is supposed to work
  - Detailed description of arguments
  - List of exceptions
- Logical structure
  - Enquiry methods (eg. GetSinglePhasePropList)
  - Check methods (eg. CheckSinglePhasePropSpec)
  - Calculate methods (eg. CalcSinglePhaseProp)



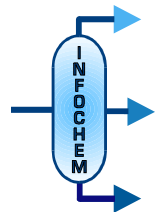
# Objectives

- Enhance functionality
  - Properties
    - Constants (pure compounds)
    - T/P-dependent properties (pure compounds)
    - single-phase mixture properties
    - 2-phase mixture properties
  - Phases
    - Any number of phases
    - Any types of phases (normally homogeneous)
  - Generalise flash specifications
- Enable/support efficient implementations



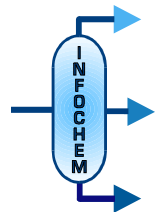
## Beyond VLE – Process modelling applications

- Mercury in natural gas/oil processing (5 phases: VLWLS)
- BP Cold Flow process - hydrates handling in sub-sea flowlines (6 phases: VLWIH1H2)
- Wax deposition in sub-sea flowlines (4 phases: VLWS)
- Polymer production (4 phases: VLLS)



# Issues with more than 2 phases

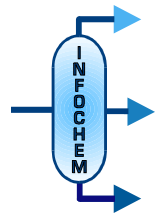
- No physical distinction between V & L phases
- Multiple liquid phases
  - how to distinguish them?
- Many possible solid phases
  - Pure solids, eg. ice, CO<sub>2</sub>
  - Fixed composition mixtures, eg. Salts
  - Semi-fixed composition mixtures, eg. Hydrates
  - Solid solutions, eg. waxes, asphaltenes
  - Non-homogeneous solids



# CO Phases

## Thermo 1.0

- Vapor
- Liquid
- Solid
- Overall
- VaporLiquid



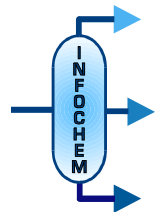
# CO Phases

## Thermo 1.0

- Vapor
- Liquid
- Solid
- Overall
- VaporLiquid

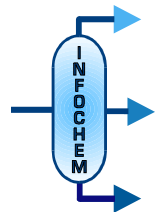
## Thermo 1.1

- Phase
  - Phase Label (identifier)
  - State of aggregation
    - Vapor, Liquid, Solid
  - Key compound id
  - Excluded compound id
  - Density description
    - Light, Heavy
  - User description
  - Type of solid
    - Pure solid, solid solution, Hydratel, Hydratell, HydrateH

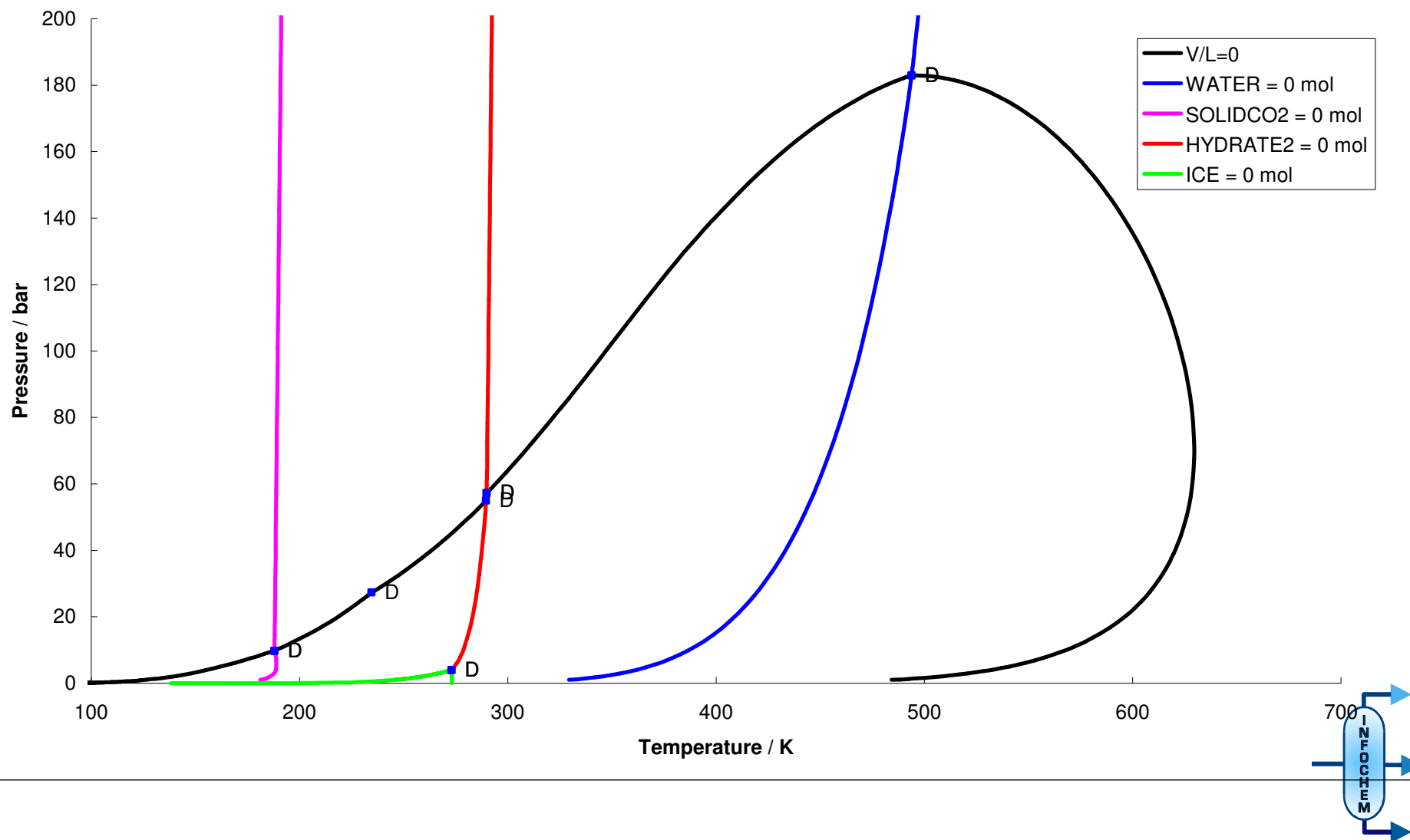


# Example – Solids dropout from Condensate

Phase Label	Gas	Liquid1	Aqueous	Ice	SolidCO2	Hydrate1	Hydrate2
State of aggregation	Vapor	Liquid	Liquid	Solid	Solid	Solid	Solid
Key comp	-	-	Water	-	-	-	-
Excluded comp	-	Water	-	-	-	-	-
Density description		Light	Heavy	-	-	-	-
User description	Gas phase	Hydrocarb on liquid	Aqueous liquid	Ice	Solid CO2	Hydrate 1	Hydrate 2
Type of solid	-	-	-	Pure	Pure	Hydrate1	Hydrate1

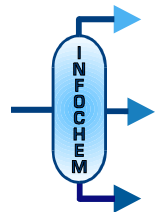


## Condensate example phase envelope



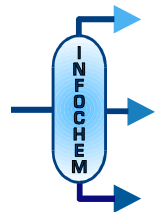
# Phase Handling (PME $\leftrightarrow$ PP)

- Identify phases
  - PME should request list of supported phases from PP and attempt to identify/reconcile them based on phase attributes
  - Produce list of phases known to PME (subset of phases supported by PP)
- Property calculation
- Phase equilibrium calculation



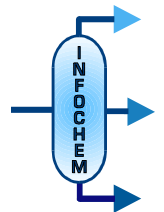
# Property calculation

- PME
  - set T,P,x for *phaseX* in MO
  - Call CalcSinglePhaseProp method on PP
- PP
  - get T,P,x for *phaseX* from MO
  - do property calculation for *phaseX*
  - set result in MO



# Phase Equilibrium Calculation

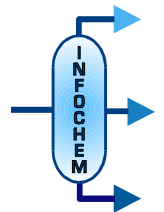
- PME
  - Specify list of phases to be considered using **SetPresentPhases** method on MO
  - Set overall composition and 2 constraints to define calculation (eg. P and T)
  - Call **CalcEquilibrium**
- PP
  - Get calculation constraint values etc. from MO
  - Get list of phases for calculation using **GetPresentPhases** method on MO
  - Do calculation
  - Use **SetPresentPhases** method to indicate the phases *actually present* at equilibrium
  - Set phase P,T,x and phase fractions in MO



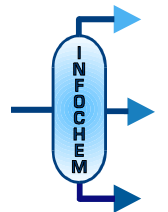
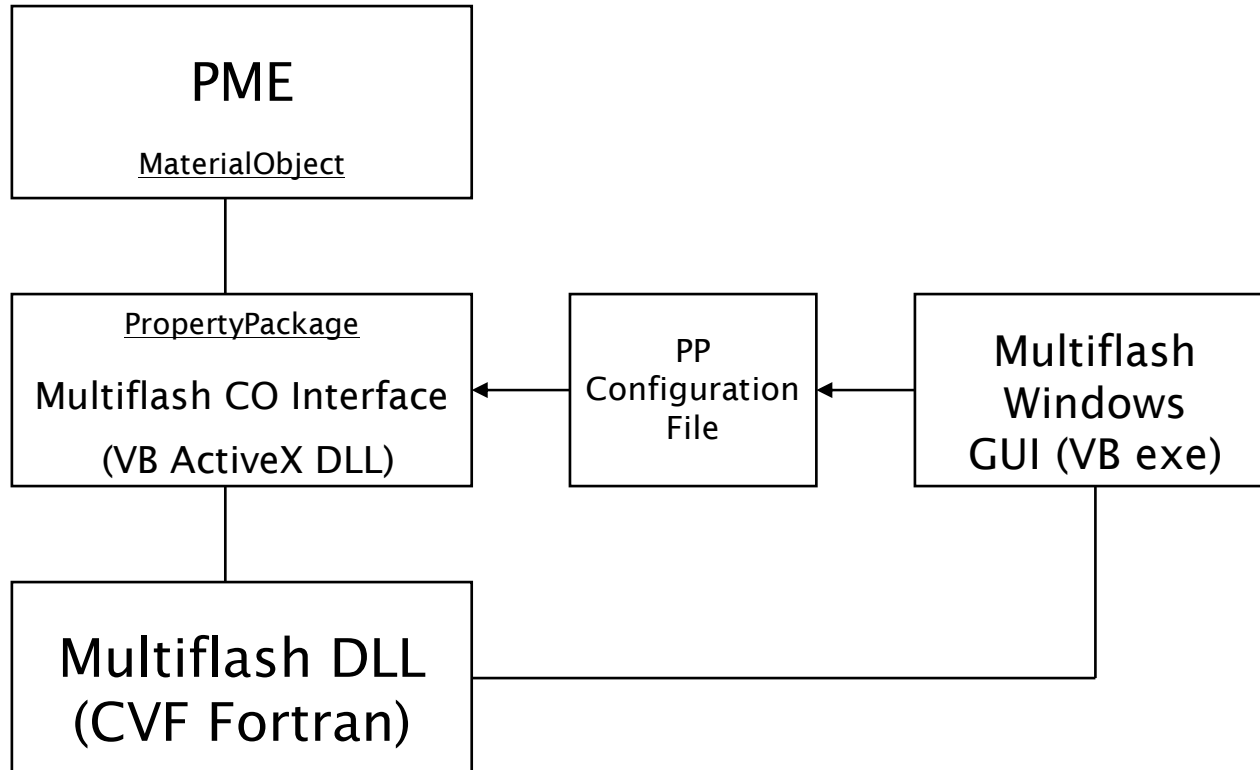
# Implementing a Thermo 1.1 PP based on Multiflash

## ■ Multiflash

- Physical property package with wide range of models for properties and phases
- multi-phase capability – no logical limit on number of fluid and/or solid phases
- Supports all flash specifications for *any* combination of phases
- Analytical derivatives of phase properties w.r.t.  $p$ ,  $T$  and composition
- Analytical derivatives of flashes w.r.t. inputs
- Packaged as Win32 dll

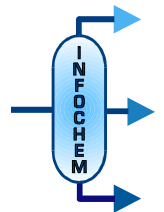


# Technical Approach



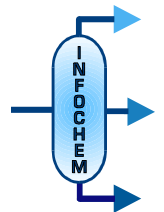
# Implementing the 1.1 Standard


- **The positive**
  - Started with the Multiflash 1.0 CO Property Package
  - Relatively straightforward to adapt and extend an existing 1.0 PP for 1.1
  - Existing code for many methods, eg. CalcProp, can be reused and greatly simplified
- **The difficulties**
  - Complexity of handling large number of flash specifications in a uniform way
  - Substantial effort implementing a MO and test environment
  - Multithreading
  - Difficult to check interoperability
  - CO Tester has not been updated to match latest revision of standard



# Summary

- Generalising phases (and flashes) makes the 1.1 interface more flexible but may require changes in the way that the PME and PP interact
- Many applications for simulations with more than 2 phases
- Relatively simple to implement Thermo 1.1 PP
- Limited interoperability experience





# Beyond VLE – a Thermo 1.1 Property Package

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