Who Knows Where the Time Goes? Computational overheads of using the thermodynamics interfaces

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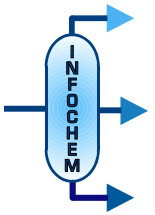
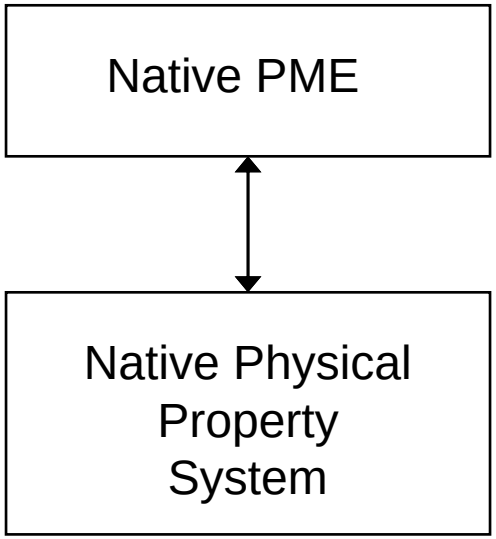
Objectives

- Determine computational overhead of using CO thermo interface compared with a native interface
- Identify how overhead is divided between different software components
- Recommendations for
  - PP developers
  - PME/application developers
  - Future CO specs
- Discussion

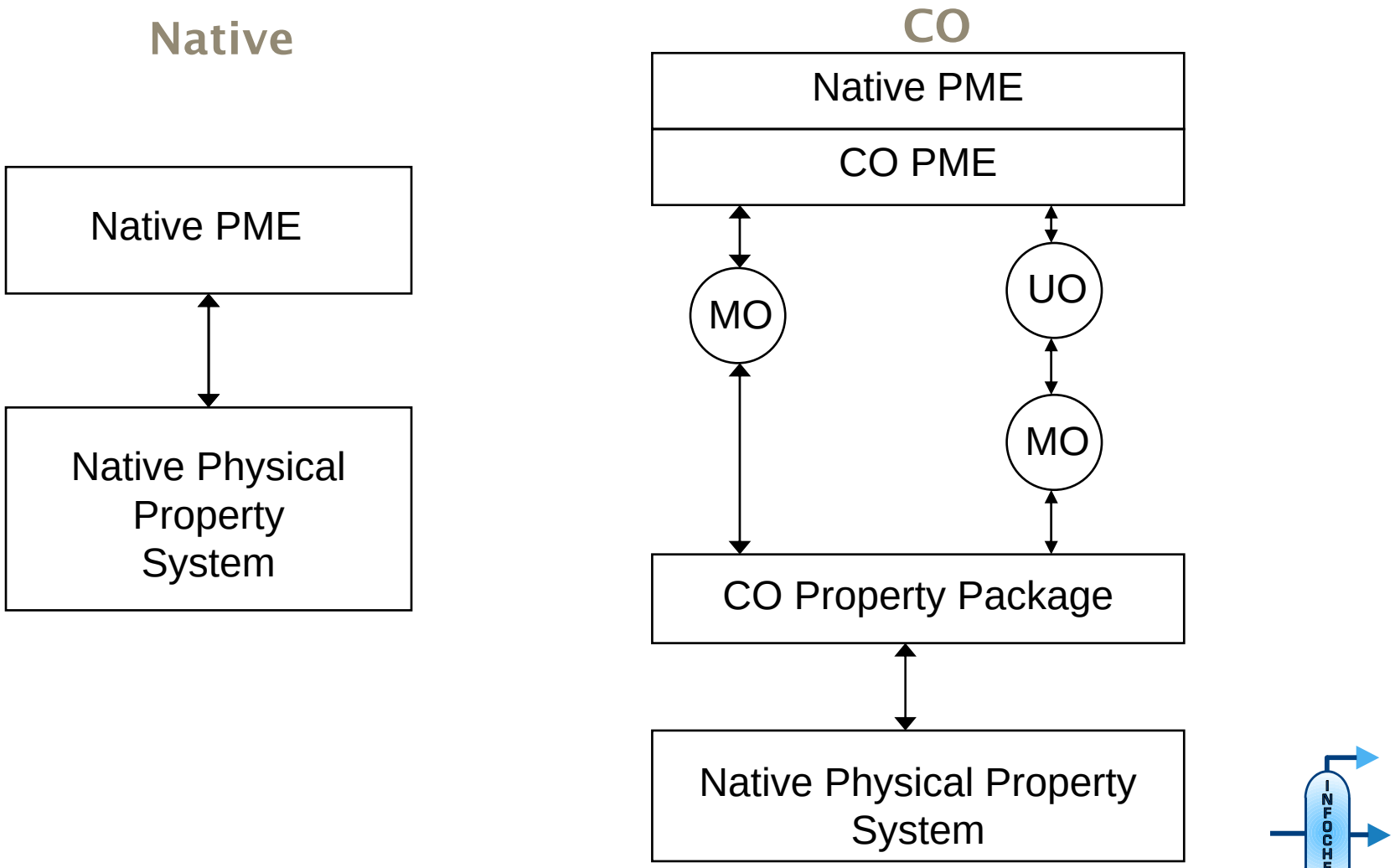


Software components

Native

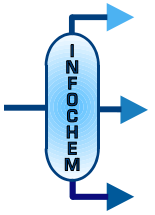


Software components



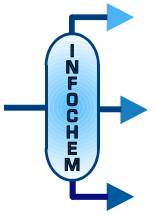
Tools Used

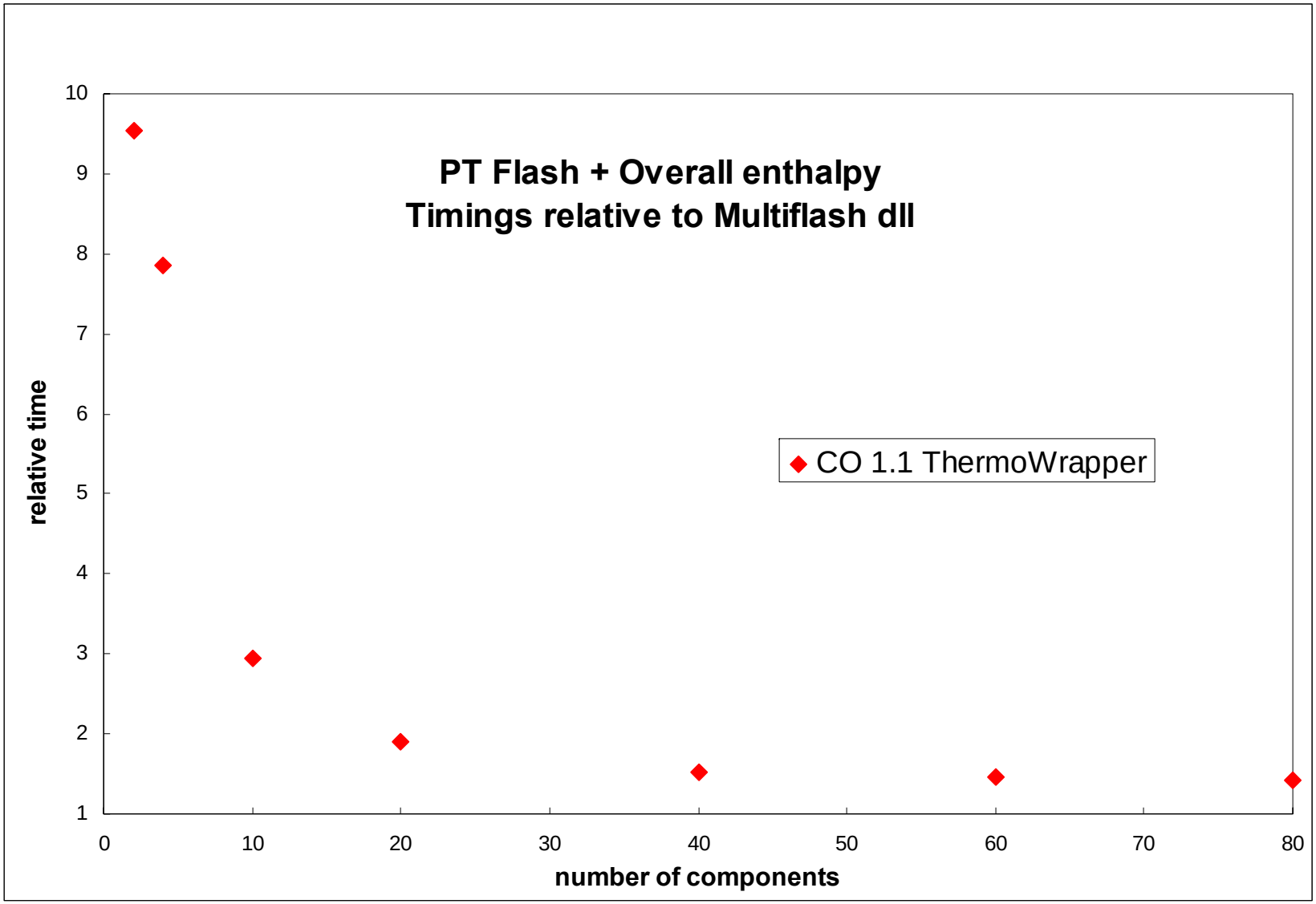
- Native physical property system
  - Multiflash 3.8 dll
  - RKS equation of state
  - Equimolar mixtures of 2 to 80 compounds (hydrocarbons)
  - Calculations over grid of P, T points with large number of repetitions
  - CP time reproducibility: 5 – 10%
- Multiflash CO Property Package
  - Implemented in C++
  - Supports CO thermo 1.0 and 1.1
- ThermoWrapper for CO 1.1
  - Library of Fortran-callable routines for using CO interfaces
  - Provides a Material Object implementation
- CO 1.0 Test Application
  - Custom application using CO 1.0 interface and MO
- Matlab CO Thermo Import (AmsterCHEM)
  - Allows a CO 1.1 PP to be imported into Matlab and used to perform physical property calculations



PT Flash & Overall Enthalpy (CO 1.1)

- Application
  - Specify MO to be used: **PP_SetMaterial**
  - Specify list of phases to be considered: **MO_SetPresentPhases**
  - Set overall composition and 2 constraints to define calculation (P and T): **MO_SetOverallProp x 3**
  - Call Property Package: **PP_CalcEquilibrium**
- PP_CalcEquilibrium
  - Get calculation conditions: **MO_GetOverallTPFraction**
  - Get list of *possible* phases for calculation: **MO_GetPresentPhases**
  - **Do (P,T) flash calculation: call Multiflash dll**
  - Set list of phases *actually present* at equilibrium: **MO_SetPresentPhases**
  - Set phase compositions,phase fractions, T, P: **MO_SetSinglePhaseProp x 4NP**
- Application
  - Get list of phases at equilibrium: **MO_GetPresentPhases**
  - Get phase fraction and composition **MO_GetSinglePhaseProp x 2NP**
  - Calculate phase enthalpy **PP_CalcSinglePhaseProp x NP**
  - Get phase enthalpy **MO_GetSinglePhaseProp x NP**




PT Flash + Overall enthalpy
Timings relative to Multiflash dll
relative time
number of components
CO 1.1 ThermoWrapper
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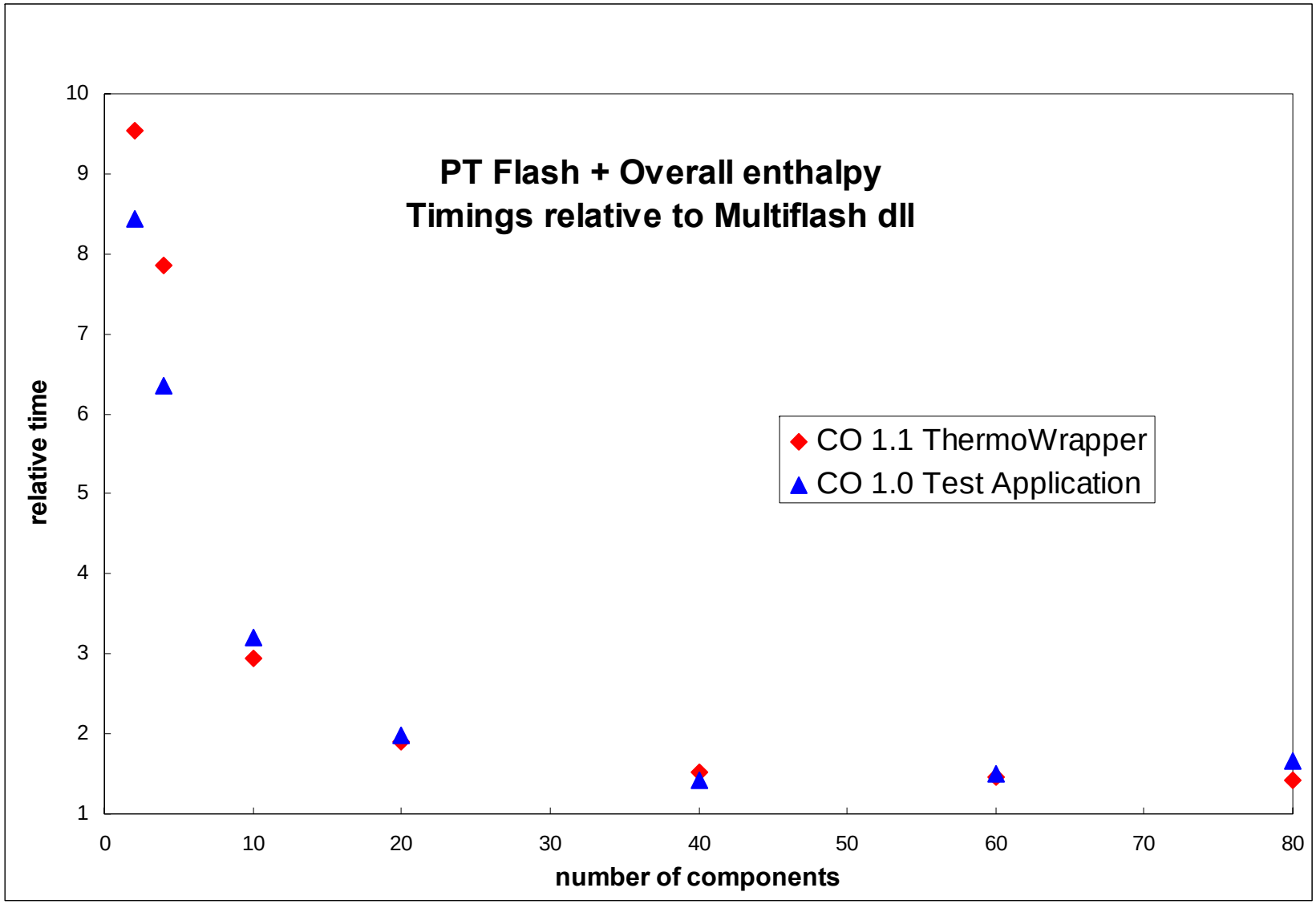
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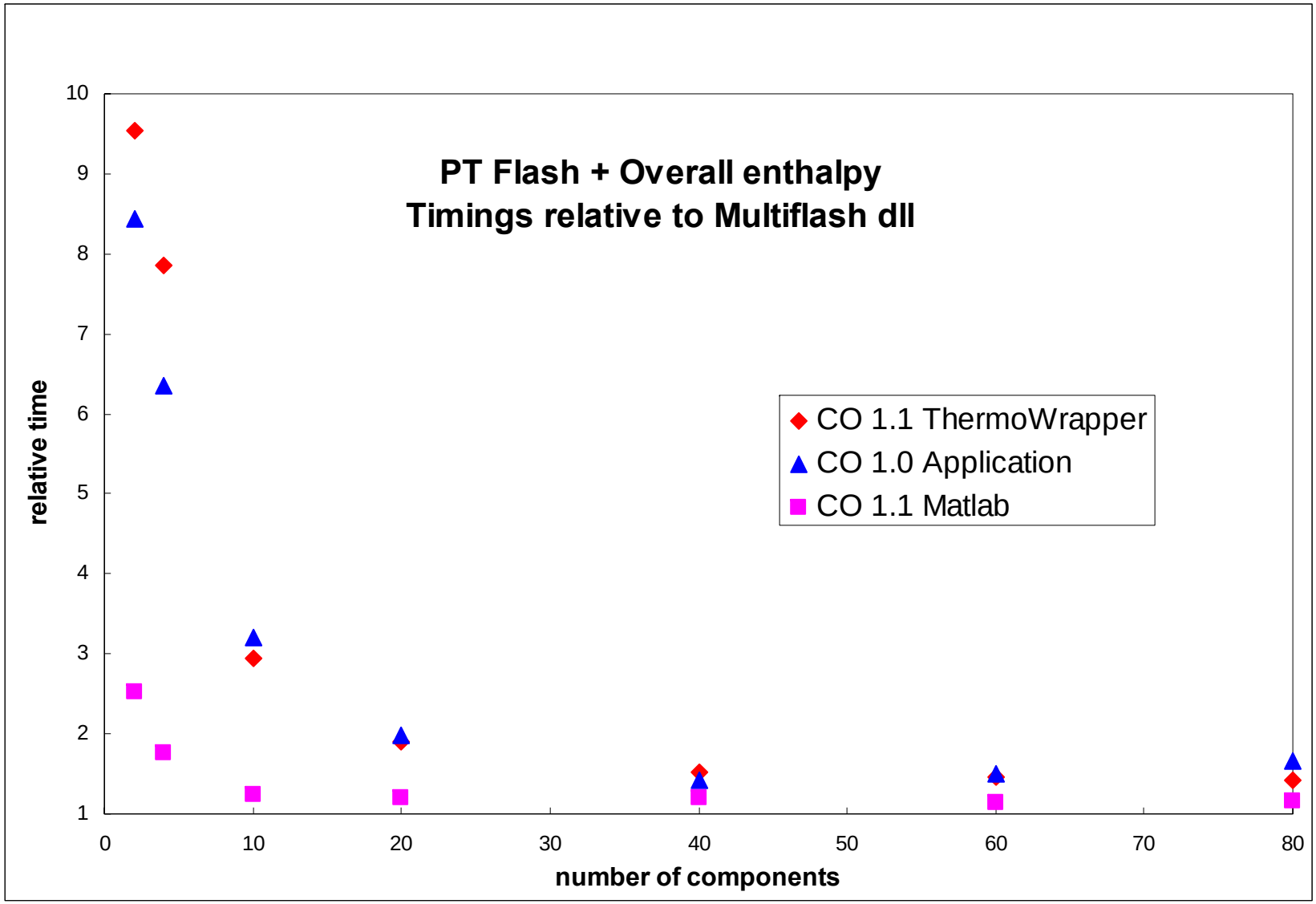
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CO 1.1 Matlab
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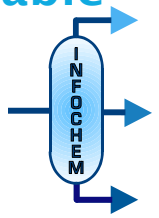
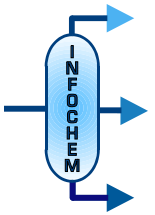
Comments

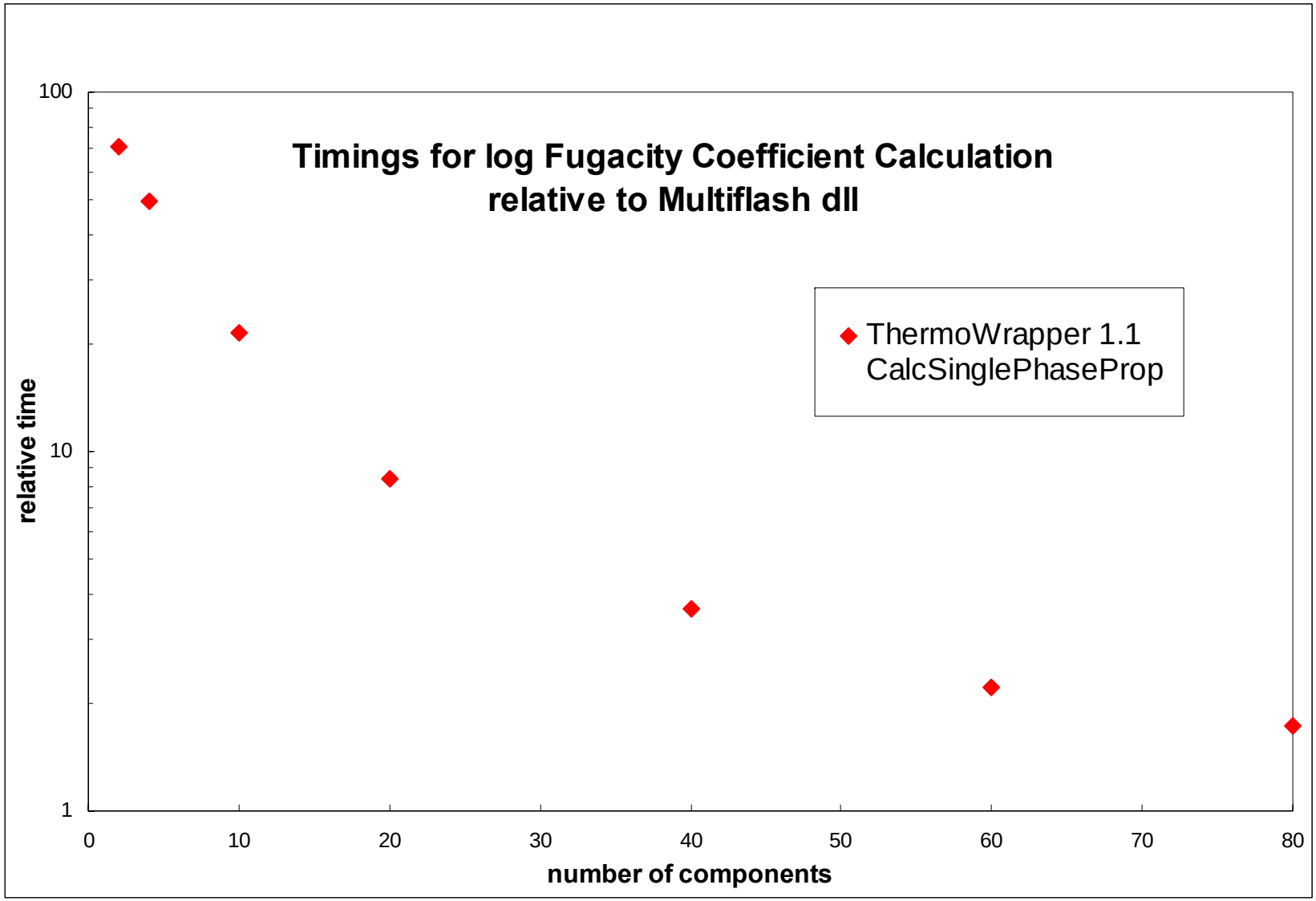
- Applications
  - ThermoWrapper: CO 1.1, Fortran, versatile MO
  - Test application: CO 1.0, C++, versatile MO
  - Matlab: CO 1.1, C++, simple MO
- Differences between 1.0 and 1.1
  - Analysis of compounds in MO
    - For 1.1 is only done when SetMaterial called
    - For 1.0 must be done on every call for a calculation
  - Getting calculation conditions
    - 1.1 has GetTPFraction and GetOverallTPFraction
  - Fewer arguments in 1.1
    - Set/Get: no compound list
    - Calculate: no calcType or MO
- Performance
  - No significant penalty for large number of compounds (>40) whatever the implementation
  - For more complex models overhead will be smaller
  - By appropriate design of MO it is possible to have a reasonable overhead even for small number of compounds



Property Calculation (CalcSinglePhaseProp)

- Application
  - Set P, T and composition of a phase: MO_SetSinglePhaseProp x 3
  - Call to Property package: PP_CalcSinglePhaseProp
- PP_CalcSinglePhaseProp
  - Get P, T and composition of phase: MO_GetTPFraction
  - Calculate property: call Multiflash dll
  - Set property value(s): MO_SetSinglePhaseProp
- Application
  - Get property value(s): MO_GetSinglePhaseProp




Timings for log Fugacity Coefficient Calculation
relative to Multiflash dll
ThermoWrapper 1.1
CalcSinglePhaseProp
relative time
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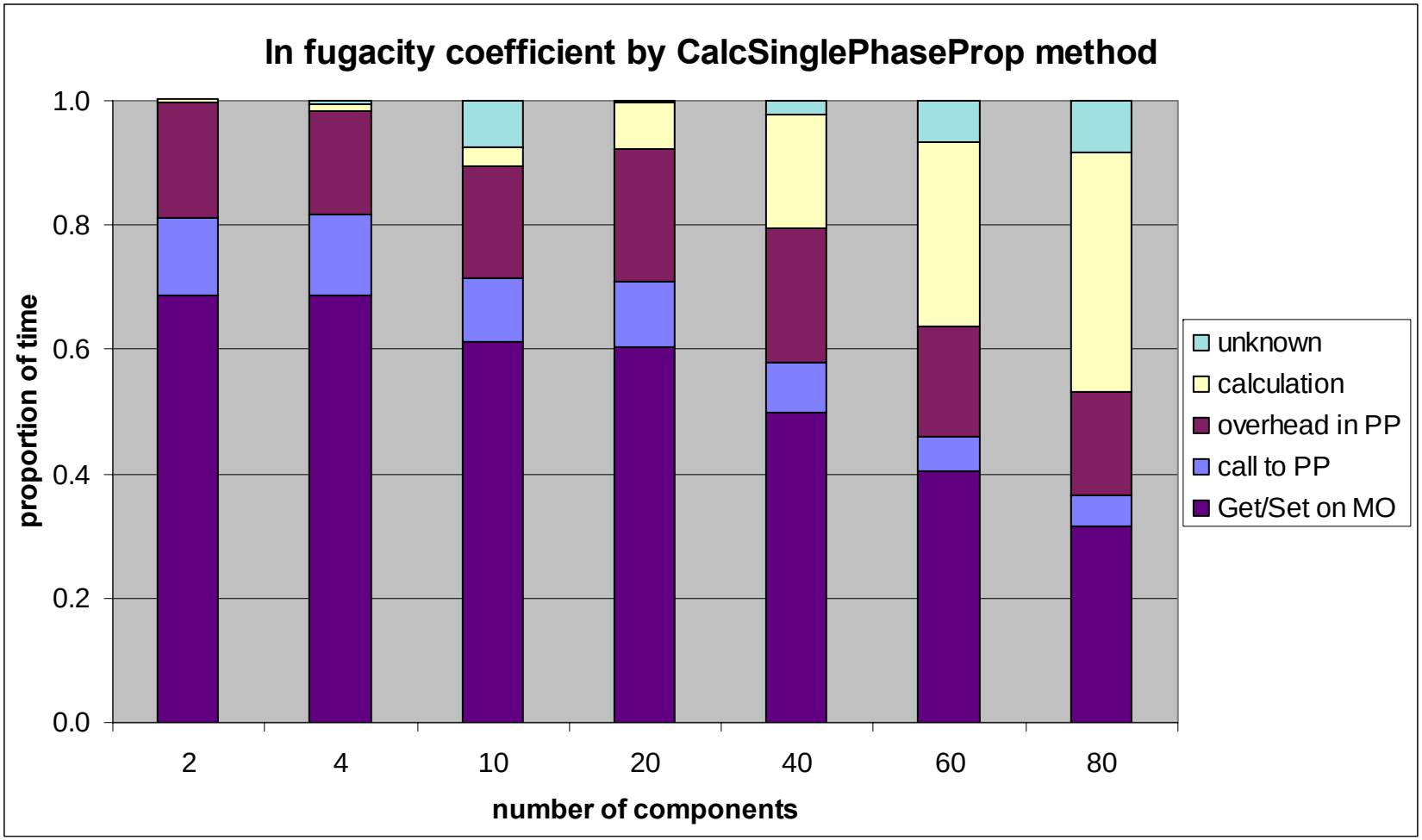
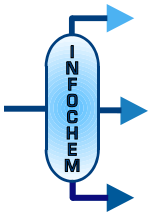
number of components

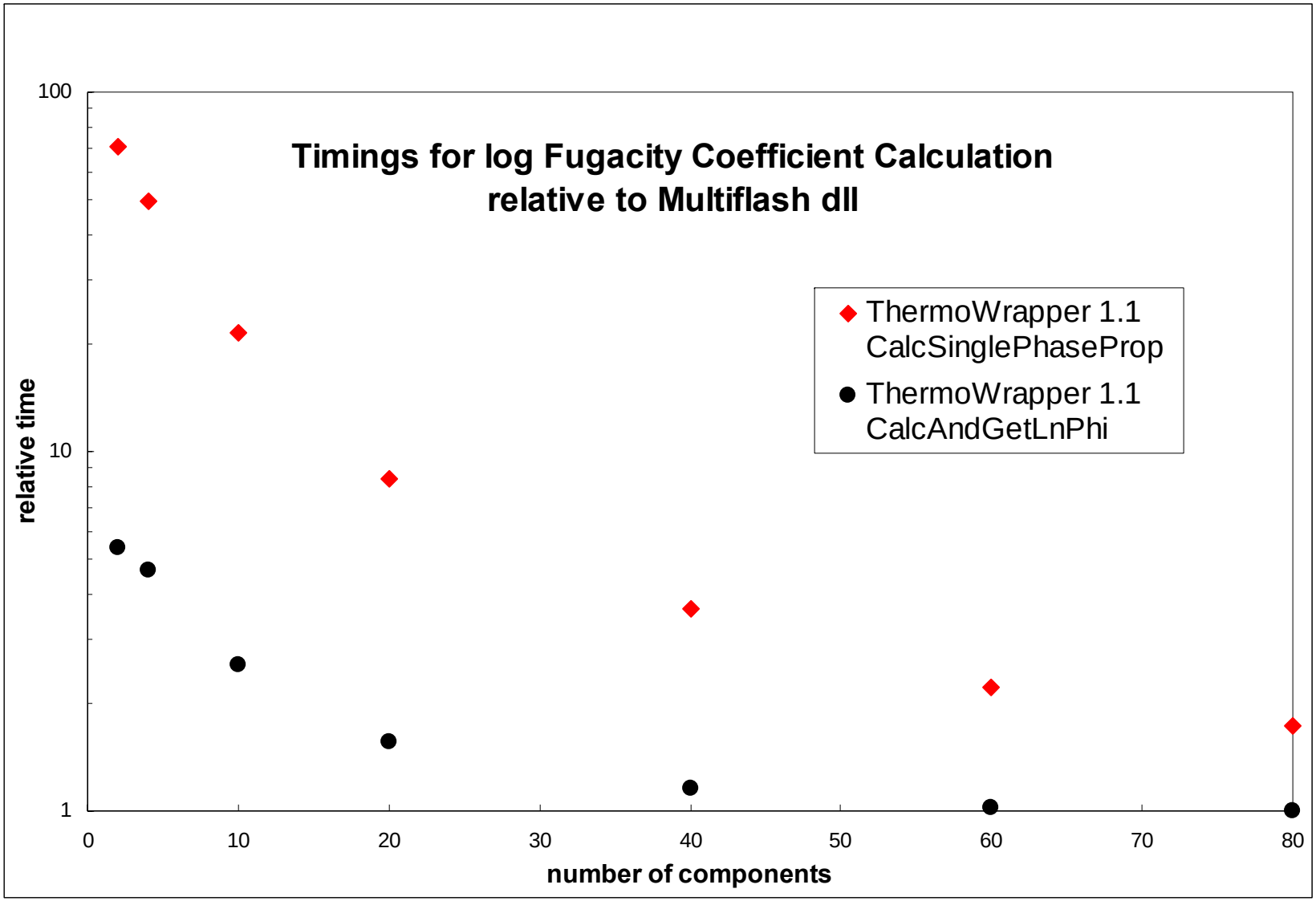
Timings for CalcSinglePhaseProp (VB PP)



Property Calculation (CalcAndGetLnPhi)

- Method does not use Material Object for communication
- PME
  - Call Property Package:
    PP_CalcAndGetLnPhi(T,P,x,lnφ)
- PP_CalcAndGetLnPhi
  - Type conversions COM to double
  - Calculate lnφ: call Multiflash dll
  - Type conversions double to COM

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ThermoWrapper 1.1
CalcAndGetLnPhi
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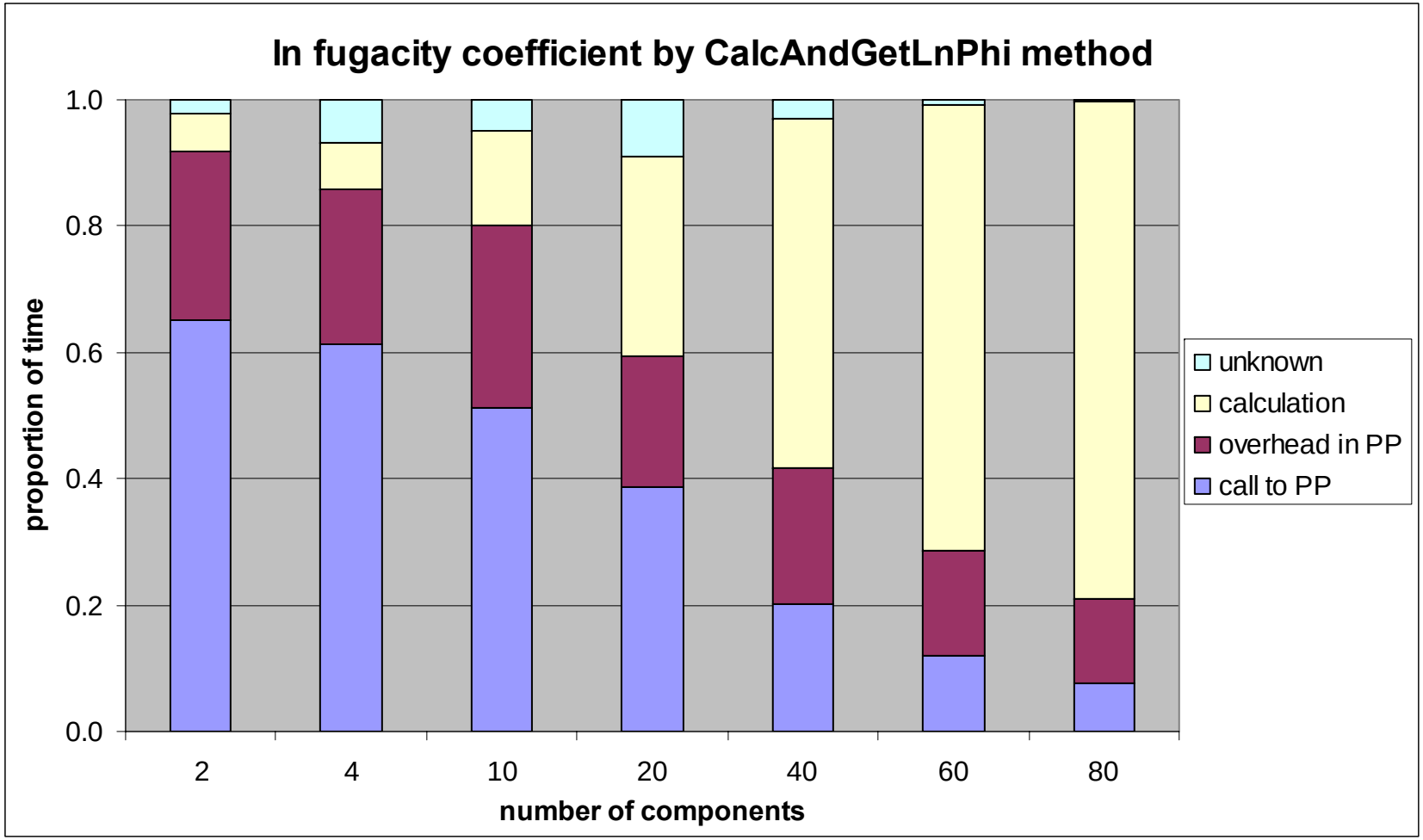
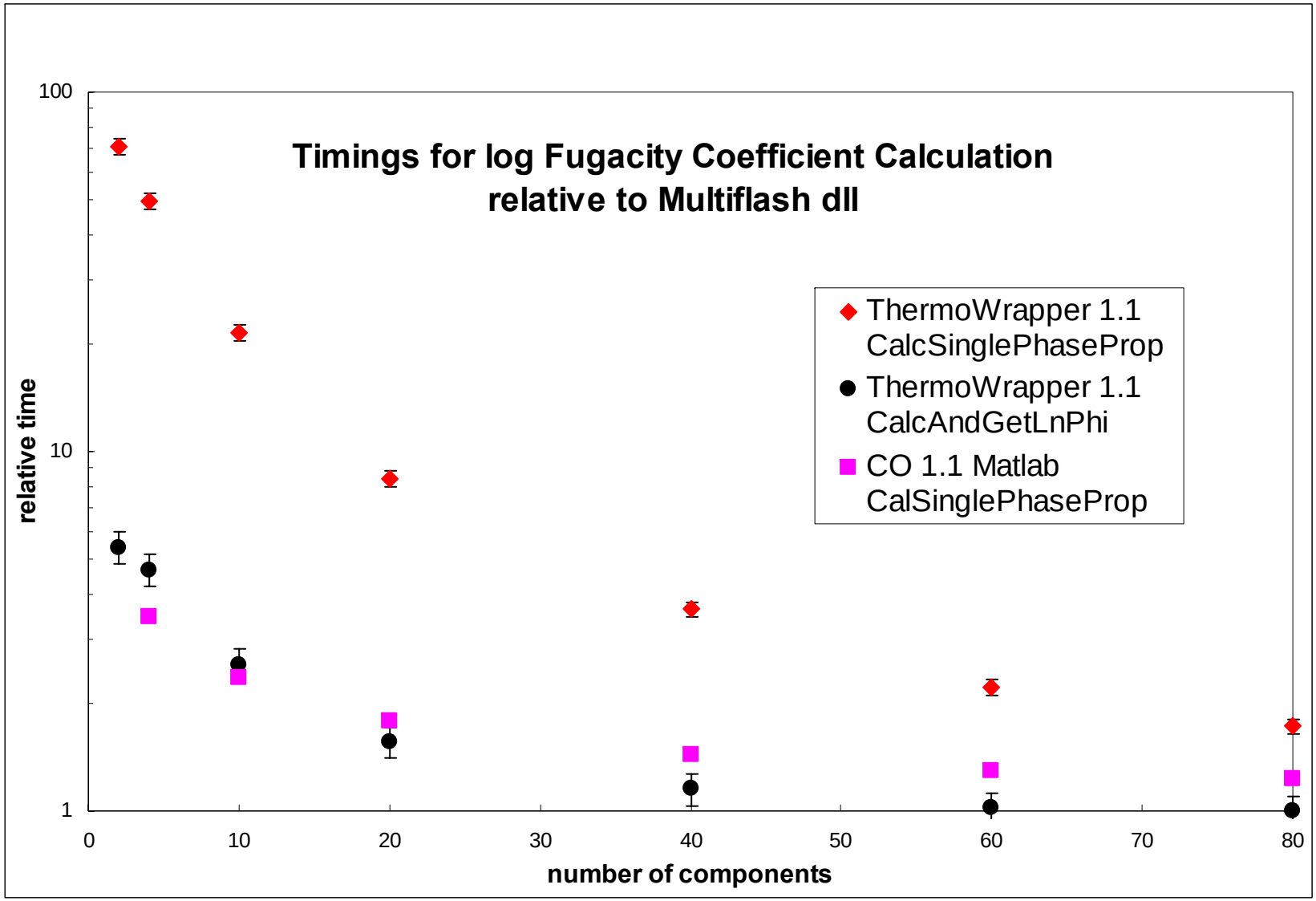
Timings for CalcAndGetLnPhi (VB PP)

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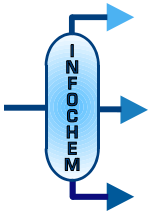
ThermoWrapper 1.1
CalcSinglePhaseProp
ThermoWrapper 1.1
CalcAndGetLnPhi
CO 1.1 Matlab
CalSinglePhaseProp

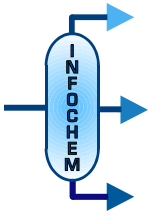
Conclusions and Recommendations 1

- The overhead of using a CO property package can be made quite small: factor of between 1 and 2
- Much of the overhead seems to be associated with the design and operation of the Material Object
  - Competing objectives of efficiency and generality
    - error checking and diagnostics
    - type conversions
    - support of both thermo 1.0 and 1.1 in the same MO
    - PME interaction with MO
  - Attend the short course on implementing MOs
- Thermo 1.1 offers the possibility of more efficient operation
  - SetMaterial
  - GetTPFraction and GetOverallTPFraction
  - Fewer arguments



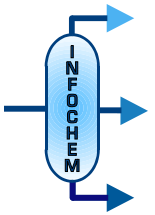
Conclusions and Recommendations 2

- PP Design is also important
  - Re-writing the Multiflash PP in C++ instead of VB reduces CalcSinglePhaseProp time by 25% for small no. of compounds, no difference for large no.
  - Essential to analyze the compound list efficiently and only when SetMaterial is called
- PME design
  - The PME should use SetMaterial only when the MO changes its compound list or compound order (or phase list for flashes)
  - PME owns the MO so can avoid all CO Set/Get calls
- Comparisons of CO and native applications for complete flowsheets would be more realistic for estimating overheads
  - However > 80% of simulation time is typically spent in phys props calculations



Conclusions and Recommendations 3

- Improvements to thermo interfaces
  - methods to identify compounds, phases and properties by integers (handles) rather than strings
  - Direct methods (similar to CalcAndGetLnPhi) for evaluating properties in order to eliminate use of MO as much as possible
  - SetTPFraction and SetOverallTPFraction methods to eliminate multiple references to MO



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