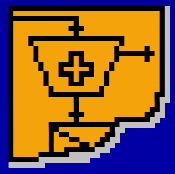

SolidSim

Flowsheet simulation of solids processes

SolidSim - A novel simulation system makes use of the CAPE-OPEN standard

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Project goals

- Development of a simulation tool for processes which involve solids

- Development of a model library for the unit operations of particle technology including machines and apparatuses

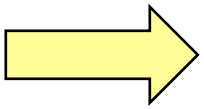
Fluid processes vs. solids processes

Fluid processes

- concentrated parameters (pressure, temperature, ...)
- complete characterization by phase equilibria, mass fractions, ...
- apparatus geometry is of minor importance

Solids processes

- distributed parameters (particle size distribution, density distribution, ...)
- characterization requires more information: shape factors, porosity, particle strength, attrition resistance, ...
- size-dependent secondary attributes: residual moisture, density, contamination, ...
- bulk properties cannot be calculated from single particles properties
- complex physical processes require consideration of apparatus geometry



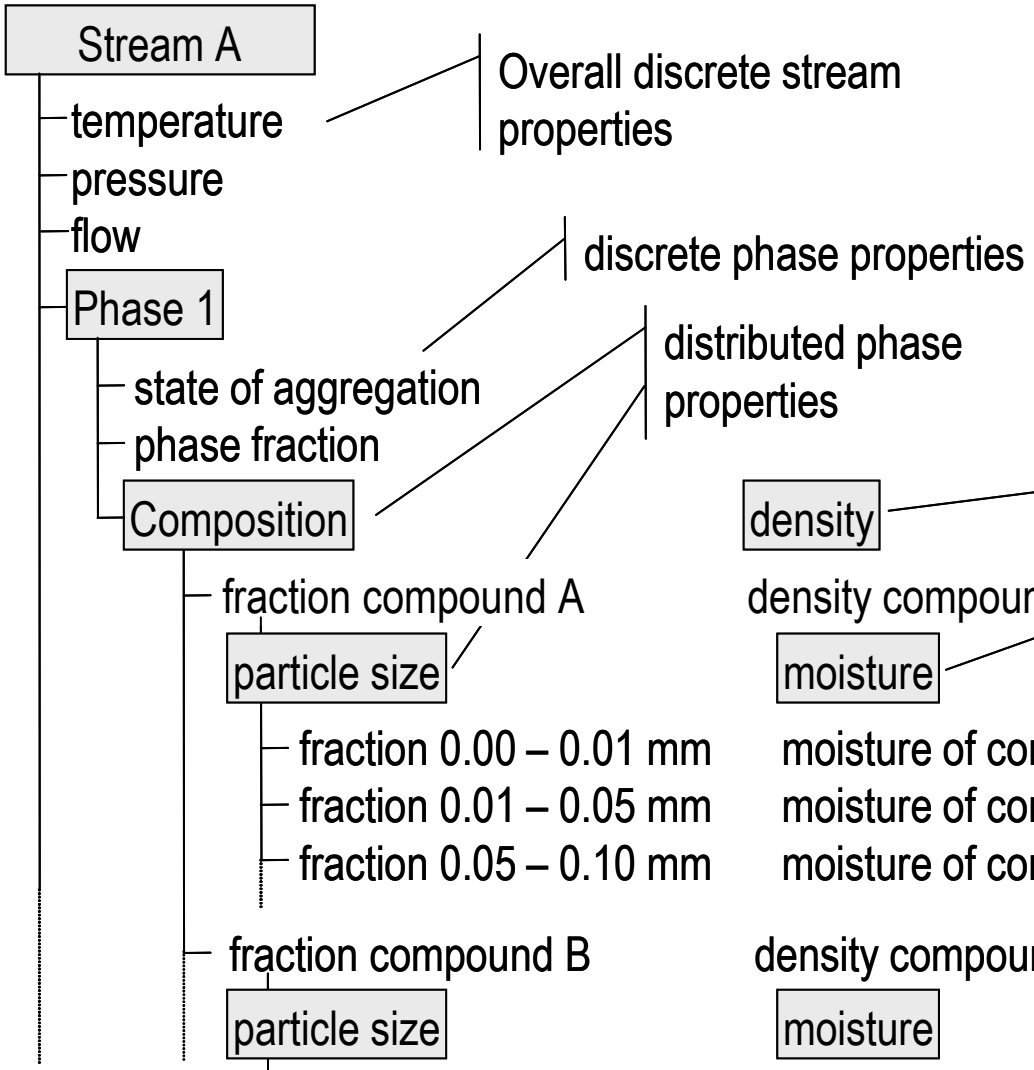
more complex structure for material objects needed

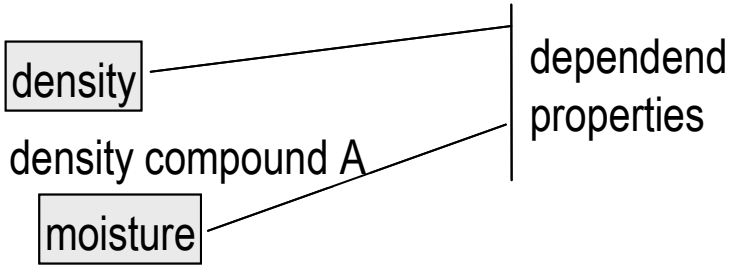
Consequences

- Due to requirements on stream structure a simple extension of existing flowsheeting systems for fluid processes with new models for solids handling is not sufficient
- A completely new system for solid-processes should be developed, which could be used
  - as a stand-alone system
  - as a base system which utilizes external models or software packages in addition to the built in models
  - as an extension for existing flow sheeting systems

A standardized interface is needed $\Rightarrow$ CAPE-OPEN

Stream definition in SolidSim





moisture of compound A with a size of 0.00 to 0.01 mm
moisture of compound A with a size of 0.01 to 0.05 mm
moisture of compound A with a size of 0.05 to 0.10 mm

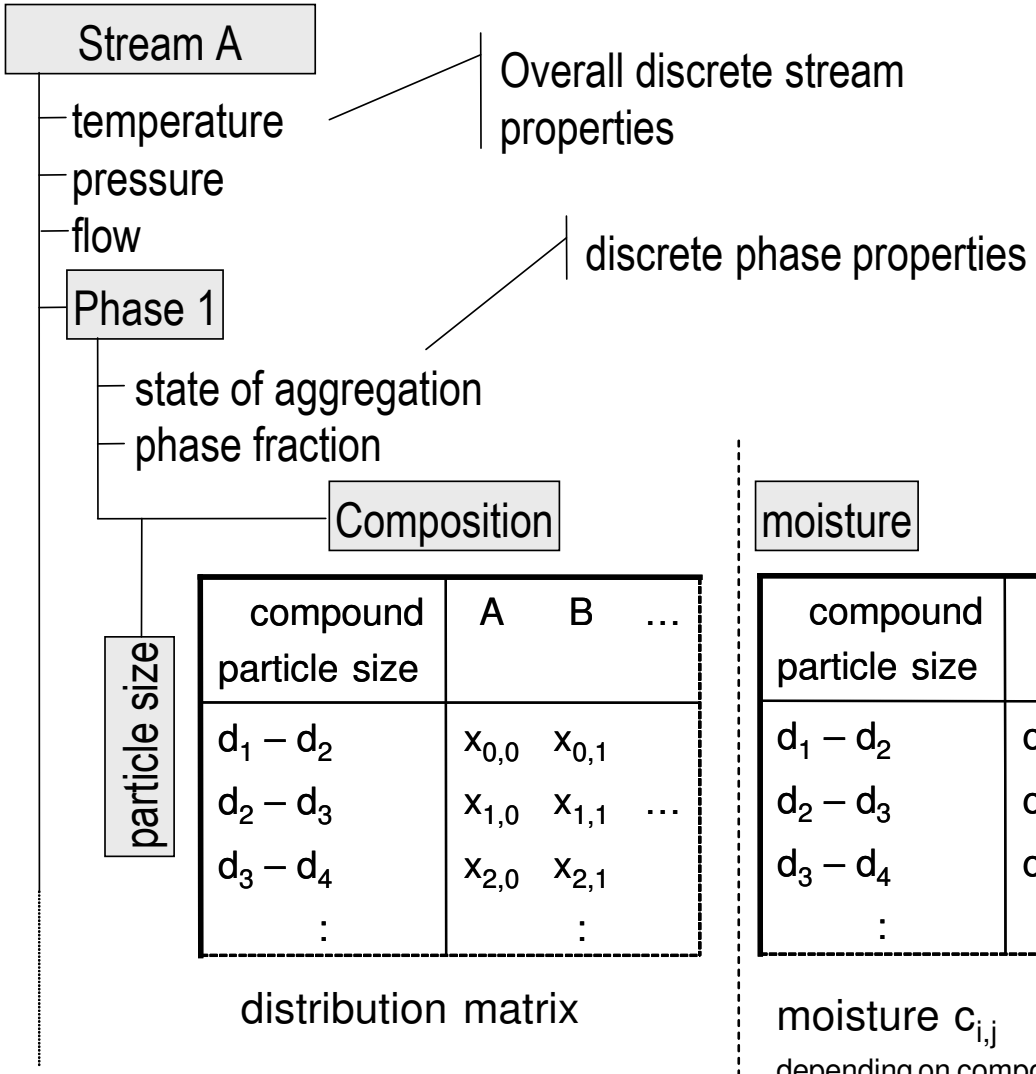
density compound B
moisture

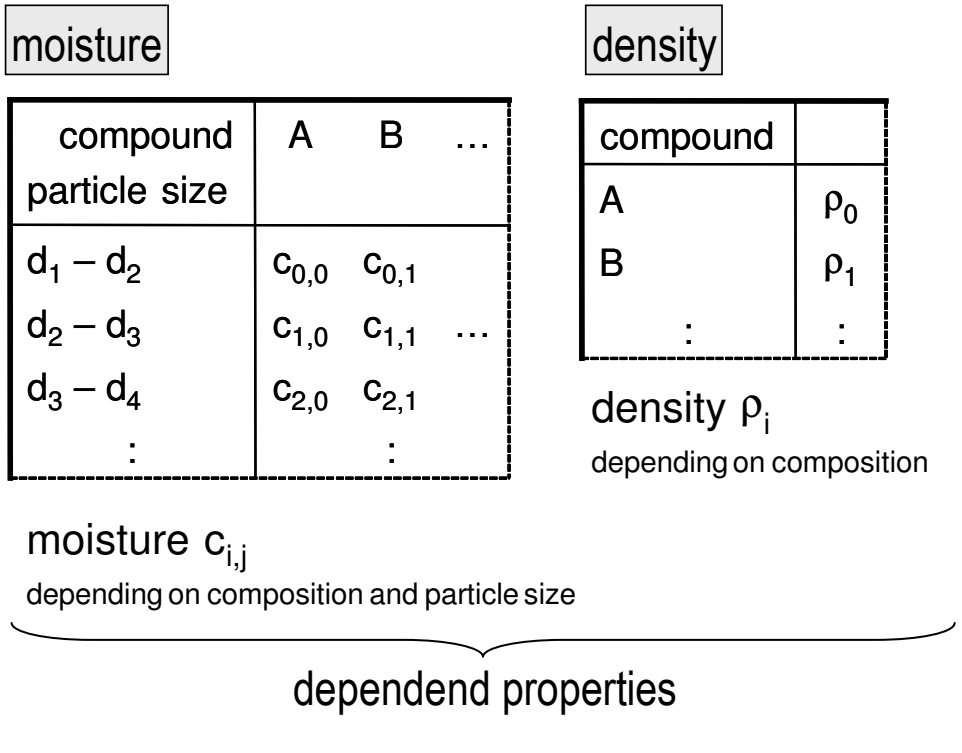
moisture of compound B with a size of 0.00 to 0.01 mm
moisture of compound B with a size of 0.01 to 0.05 mm
moisture of compound B with a size of 0.05 to 0.10 mm

Requirements:

- fast access to individual distribution of each defined attribute
- fast access to cumulated and/or mean values
- access to dependent distributions with arbitrary hierarchies

Stromdefinition in SolidSim





Requirements:

- fast access to individual distribution of each defined attribute
- fast access to cumulated and/or mean values
- access to dependent distributions with arbitrary hierarchies

Handling of distributed parameters

- To ensure correct treatment of secondary parameters it is necessary that
  - Unit Model copies input stream(s) to output stream(s)
  - Unit Model requests from stream the distribution of any attribute needed, e.g. particle size distribution (PSD)
  - Material Stream object extracts and/or calculates (usually 1-dimensional) distribution from n-dimensional matrix of attributes
  - Unit Model sets up transformation matrices for all output streams
  - Material Stream objects apply transformation matrices

Application of the transformation matrix

old property definition (stream object)

particle size

density	0	1	2	3	4	5
0	$X_{0,0}$	$X_{1,0}$	$X_{2,0}$	$X_{3,0}$	$X_{4,0}$	$X_{5,0}$
1	$X_{0,1}$	$X_{1,1}$	$X_{2,1}$	$X_{3,1}$	$X_{4,1}$	$X_{5,1}$
2	$X_{0,2}$	$X_{1,2}$	$X_{2,2}$	$X_{3,2}$	$X_{4,2}$	$X_{5,2}$
3	$X_{0,3}$	$X_{1,3}$	$X_{2,3}$	$X_{3,3}$	$X_{4,3}$	$X_{5,3}$
4	$X_{0,4}$	$X_{1,4}$	$X_{2,4}$	$X_{3,4}$	$X_{4,4}$	$X_{5,4}$
PSD	$\sum X_{0,j}$	$\sum X_{1,j}$	$\sum X_{2,j}$	$\sum X_{3,j}$	$\sum X_{4,j}$	$\sum X_{5,j}$

movement matrix for PSD (returned by unit model)

to interval

from interval	0	1	2	3	4	5
0	$T_{0,0}$	$T_{1,0}$	$T_{2,0}$	$T_{3,0}$	$T_{4,0}$	$T_{5,0}$
1	$T_{0,1}$	$T_{1,1}$	$T_{2,1}$	$T_{3,1}$	$T_{4,1}$	$T_{5,1}$
2	$T_{0,2}$	$T_{1,2}$	$T_{2,2}$	$T_{3,2}$	$T_{4,2}$	$T_{5,2}$
3	$T_{0,3}$	$T_{1,3}$	$T_{2,3}$	$T_{3,3}$	$T_{4,3}$	$T_{5,3}$
4	$T_{0,4}$	$T_{1,4}$	$T_{2,4}$	$T_{3,4}$	$T_{4,4}$	$T_{5,4}$
5	$T_{0,5}$	$T_{1,5}$	$T_{2,5}$	$T_{3,5}$	$T_{4,5}$	$T_{5,5}$

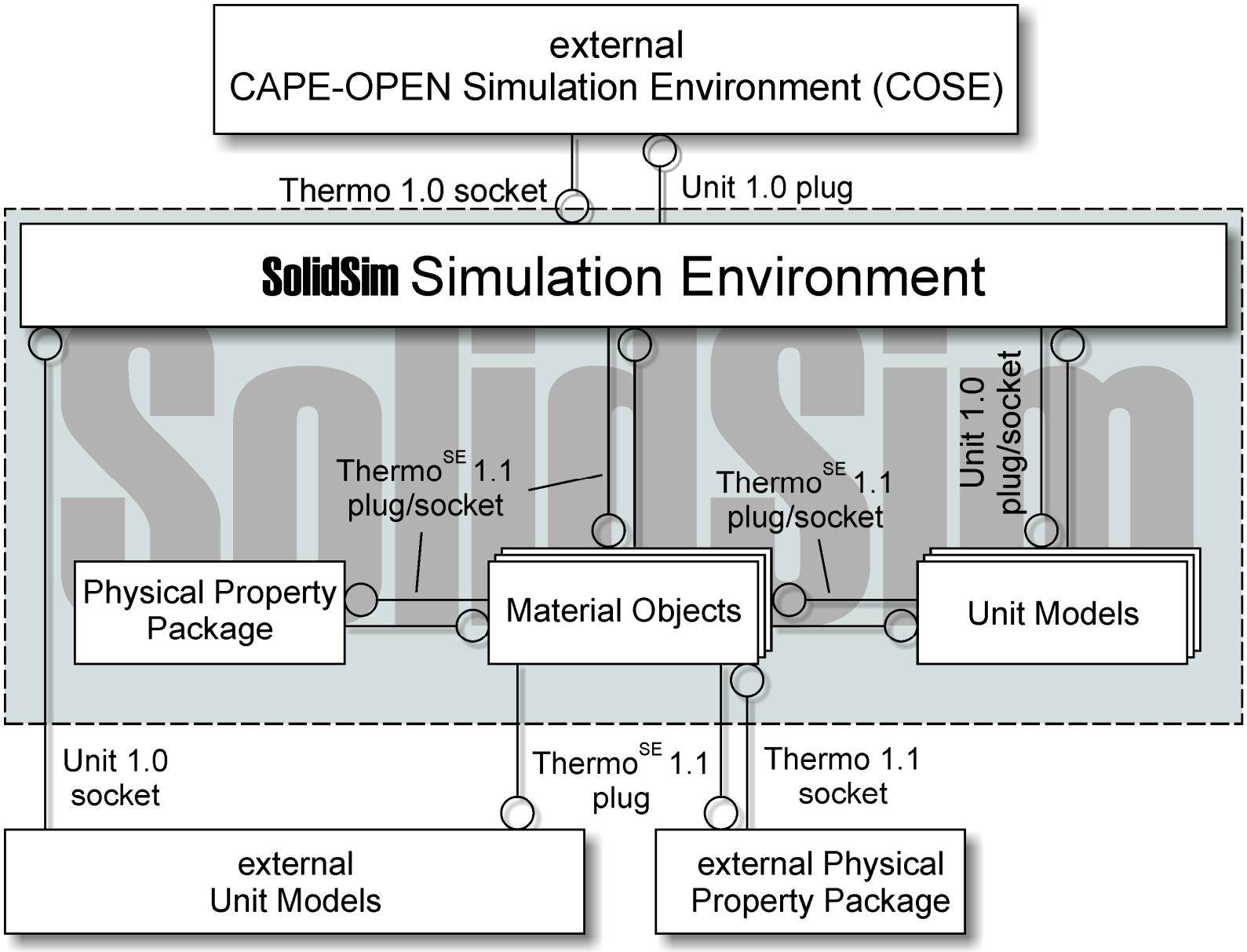
$$X'_{i,j} = \sum_k X_{k,j} \cdot T_{i,k}$$

new property definition (stream object)

particle size

density	0	1	2	3	4	5
0	$X'_{0,0}$	$X'_{1,0}$	$X'_{2,0}$	$X'_{3,0}$	$X'_{4,0}$	$X'_{5,0}$
1	$X'_{0,1}$	$X'_{1,1}$	$X'_{2,1}$	$X'_{3,1}$	$X'_{4,1}$	$X'_{5,1}$
2	$X'_{0,2}$	$X'_{1,2}$	$X'_{2,2}$	$X'_{3,2}$	$X'_{4,2}$	$X'_{5,2}$
3	$X'_{0,3}$	$X'_{1,3}$	$X'_{2,3}$	$X'_{3,3}$	$X'_{4,3}$	$X'_{5,3}$
4	$X'_{0,4}$	$X'_{1,4}$	$X'_{2,4}$	$X'_{3,4}$	$X'_{4,4}$	$X'_{5,4}$

Structure of SolidSim

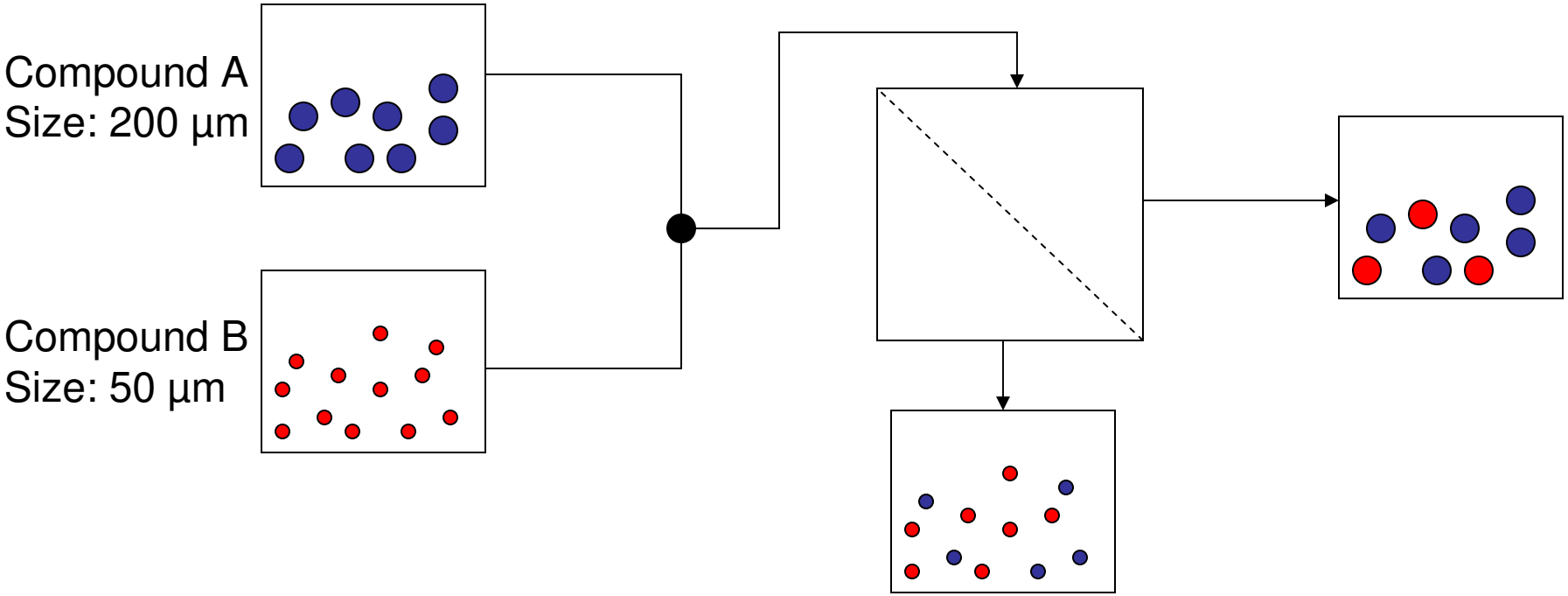


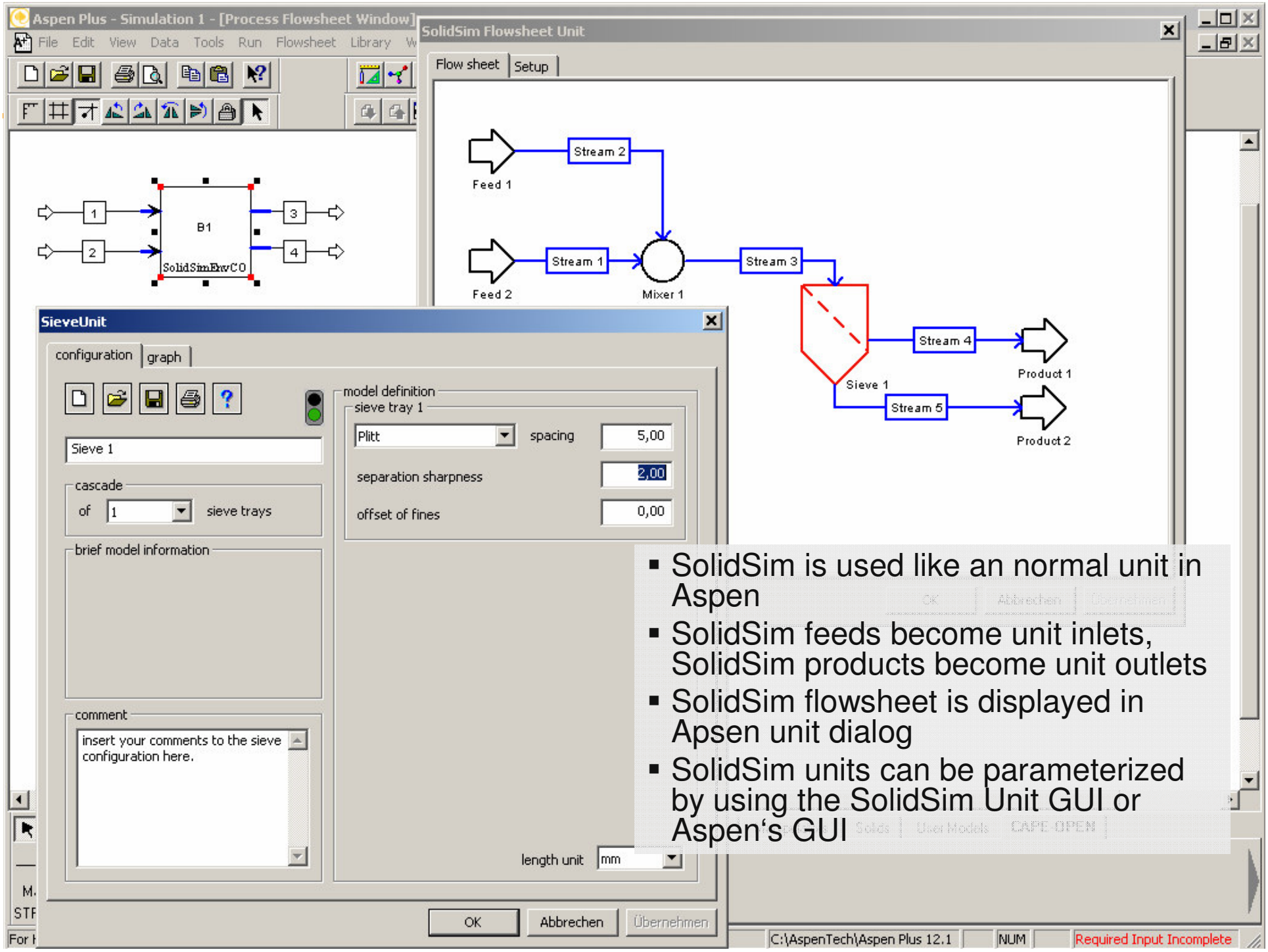
Implemented CAPE-OPEN standards

- Internally the CAPE-OPEN Thermo 1.1 standards are used, the thermo interface with the proposed extension for distributed parameters
  - SolidSim unit model
    - Thermo^{SE} 1.1 socket (requiring solids extension)
    - Unit 1.0 plug
  - SolidSim material object
    - Thermo^{SE} 1.1 plug (with solids extension)
    - Thermo^{SE} 1.1 socket
  - SolidSim PP
    - Thermo^{SE} 1.1 plug (with solids extension)
    - Thermo^{SE} 1.1 socket
- SolidSim Simulation Environment
  - Thermo 1.1 socket/plug → use of external 1.1 compliant PPs
  - Thermo 1.0 socket / Unit 1.0 plug → use of SolidSim as unit model
  - Thermo 1.1 plug / Unit 1.0 socket → use of external unit models
- SolidSim PP 1.0 Connector
  - Thermo 1.1 socket → use of external 1.0 compliant PPs
  - Thermo 1.0 plug

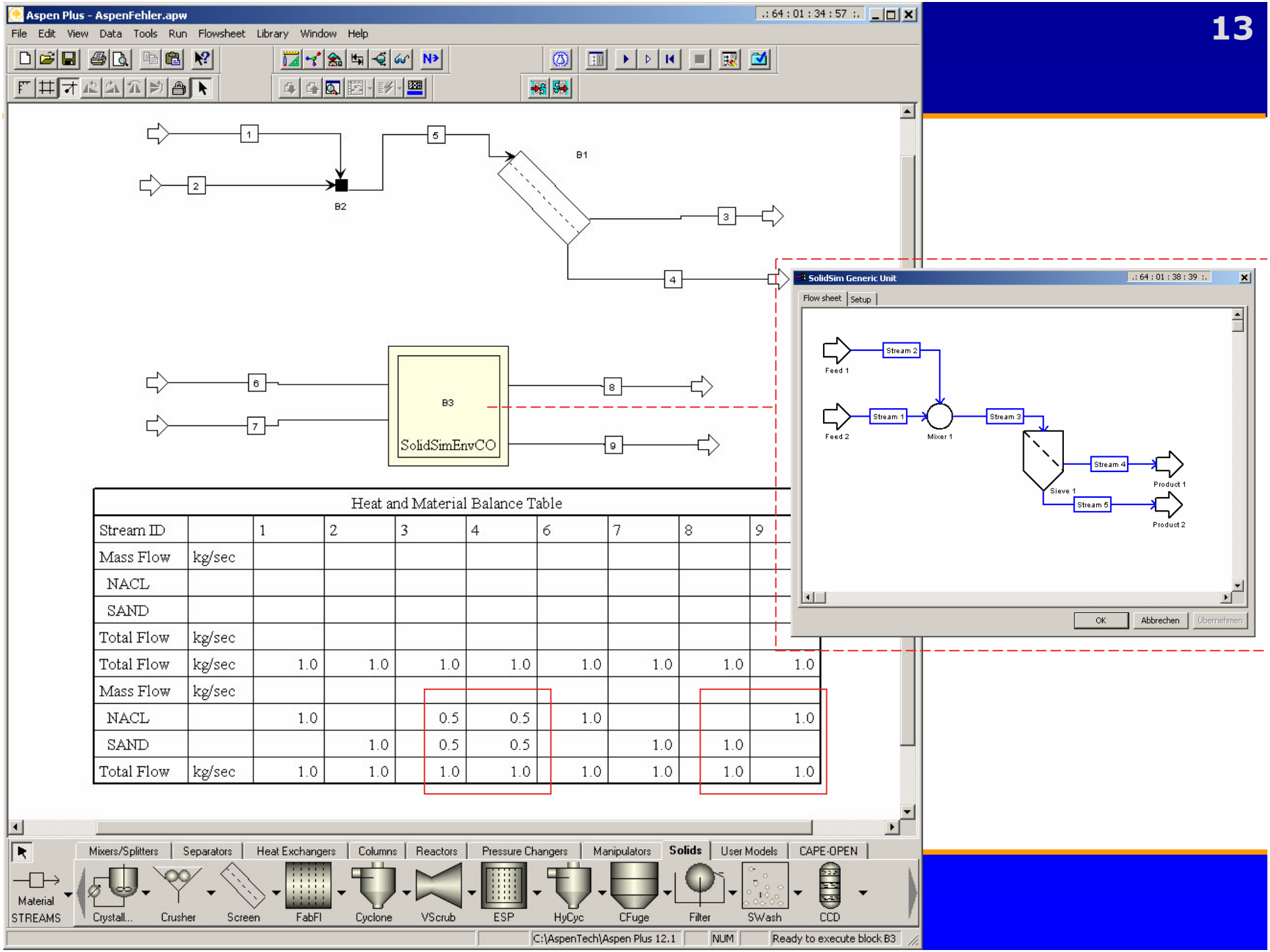
Simulation of solids processes using commercially available simulators

- Simulation software used for fluid processes can not be adopted for solids processes because of inadequate stream structure
  - Example: fraction and size information not linked





- SolidSim is used like an normal unit in Aspen
- SolidSim feeds become unit inlets, SolidSim products become unit outlets
- SolidSim flowsheet is displayed in Apsen unit dialog
- SolidSim units can be parameterized by using the SolidSim Unit GUI or Aspen‘s GUI



Heat and Material Balance Table

Stream ID		1	2	3	4	6	7	8	9
Mass Flow	kg/sec								
NACL									
SAND									
Total Flow	kg/sec								
Total Flow	kg/sec	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
Mass Flow	kg/sec								
NACL		1.0		0.5	0.5	1.0			1.0
SAND			1.0	0.5	0.5		1.0	1.0	
Total Flow	kg/sec	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0

Integration of commercial physical property packages

- Integration of commercial physical property packages allows:
  - access to external PPP's functions for calculation of:
    - transport properties (e.g. specific heat, viscosity)
    - thermodynamic properties (e.g. enthalpy, compressibility factor)
    - phase equilibria (VLE, LLE,…)
  - access to external PPP's thermodynamic model library (e.g. equation of state, activity coefficients)
  - access to pure component database

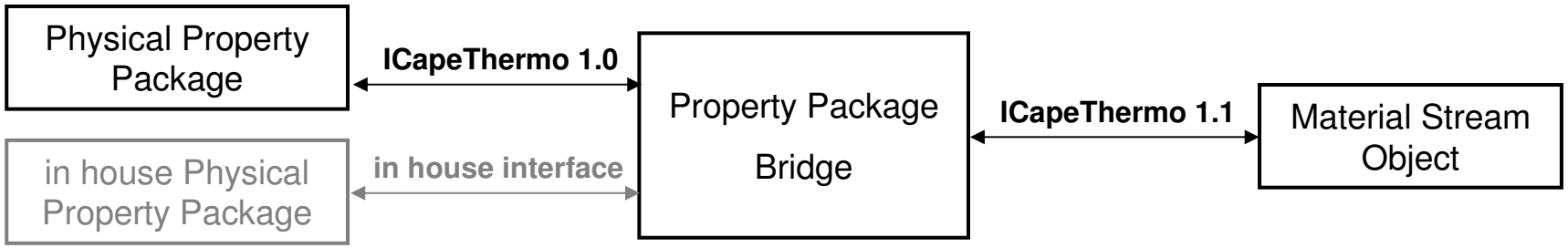
Integration of commercial physical property packages

Integration via CAPE-OPEN

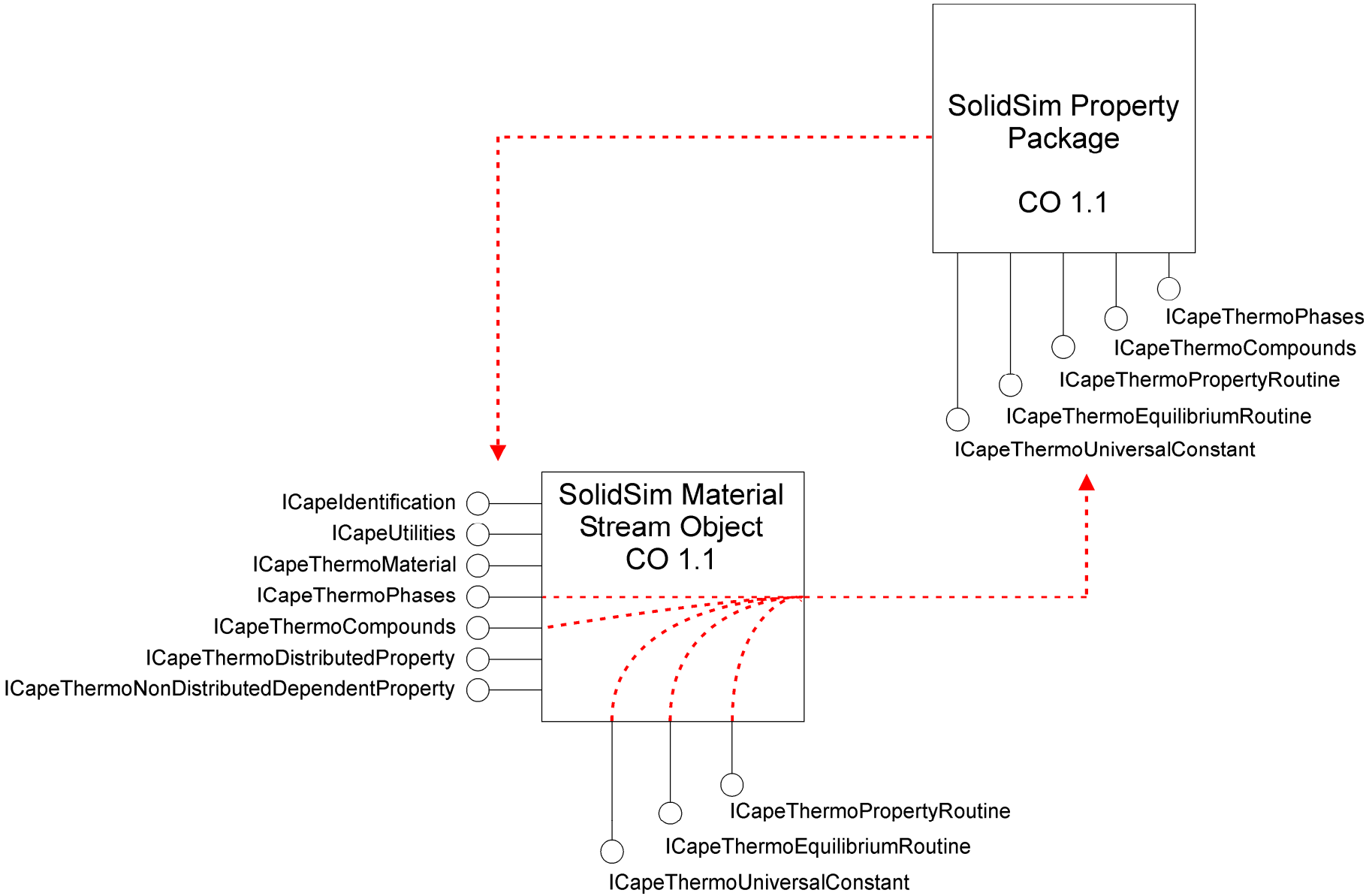
- CAPE-OPEN compliant physical property packages
  - Aspen Properties® (CAPE-OPEN Thermo 1.0)
  - Simulis® Thermodynamics (CAPE-OPEN Thermo 1.0)
  - Infochem MultiFlash® (CAPE-OPEN Thermo 1.0 and 1.1)
  - TUV - NEL PPDS (CAPE-OPEN Thermo 1.0)

- The SolidSim material stream is CAPE-OPEN compliant to CAPE-OPEN Thermo 1.1

  → Development of a software component that translates different interfaces to ICapeThermo 1.1 (Property Package Bridge)



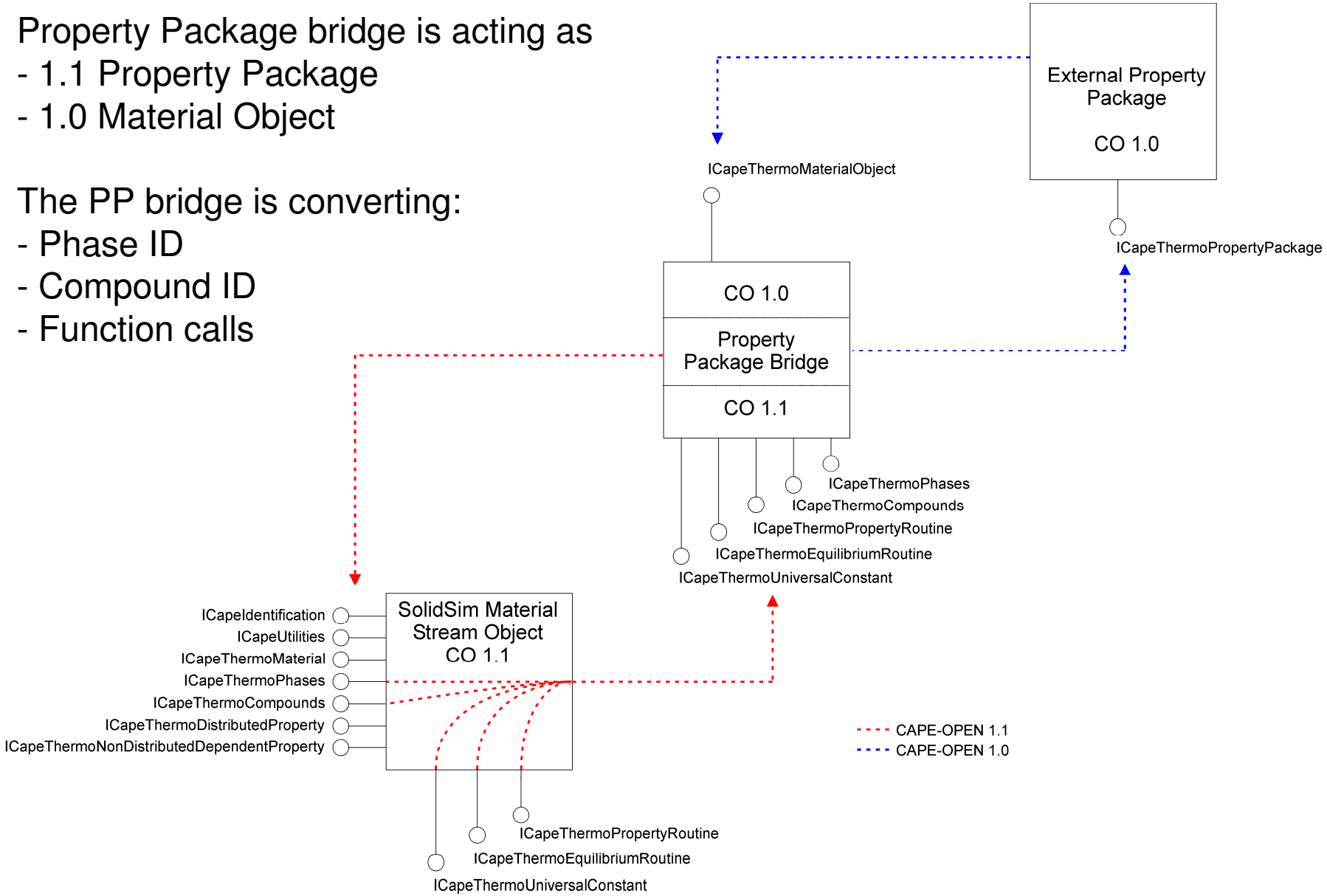
Connection to 1.1 Property Package



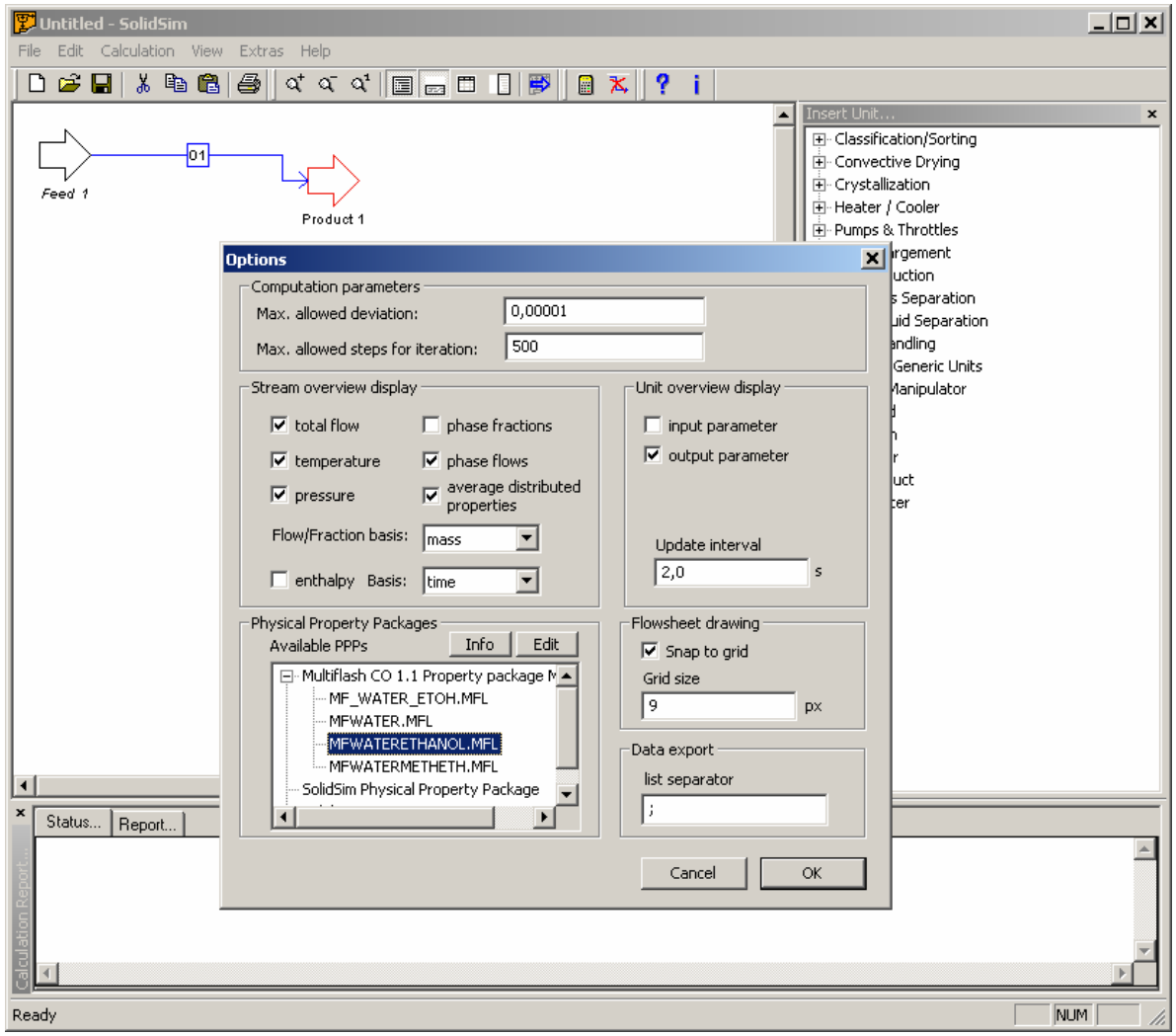
Connection to 1.0 Property Package

Property Package bridge is acting as
- 1.1 Property Package
- 1.0 Material Object

The PP bridge is converting:
- Phase ID
- Compound ID
- Function calls



Demo: SolidSim



Implemented CAPE-OPEN standards

- Internally the CAPE-OPEN 1.1 standards are used, the thermo interface with the proposed extension for distributed parameters (ICapeDistributedProperty)
- external Property Packages according to CAPE-OPEN 1.1 can be directly connected
- for use in an external COSE the SolidSim environment can be wrapped with a CAPE-OPEN 1.0 layer
  - solids related part of the flowsheet has to be modeled in the SolidSim environment
  - information about secondary attributes of solids are lost at interface streams between SolidSim and Aspen Plus
    - number of interface streams should be minimized