SolidSim

CO-LaN Meeting in Leipzig-Schkopau

The SolidSim Project

Development of a Flowsheeting Tool for Solids Processes

Outline

- The SolidSim Project
  - Project introduction
  - Design concept of Simulation Software
- CAPE-OPEN and SolidSim
- Demonstration of SolidSim

Motivation

- Flowsheet simulator for solids processes allows
  - development of flowsheets for complex processes
  - design studies for process alternatives
  - sensitivity analysis for process parameters
  - fast and easy optimization of processes involving solids
- Establish a model library for solids processing equipment and unit operations
- Support education of chemical engineering students

Comparision - Simulation of …

- Liquid/gas process
  - concentrated variables
    (temp., pressure, mass fraction)
  - complete characterization by few parameters
    (temp., composition, pressure)
  - models cover mass transfer and reactions
  - equipment geometry plays minor role in modeling
    (just influence on residence time)
  - throughput influences only residence time

- Solids processing
  - additional distributed parameters
    (particle size distr., density distr.)
  - characterization requires more parameters
    (shape factor, size distribution, porosity, breaking behaviour, etc.)
  - partially dependant secondary attributes
    (particle size dep. composition (ore) or moisture content, surface area dependant contamination)
  - model has to account for very complex physical effects
    (e.g. impact mill, dryer, fluidized bed)
    - most models only valid for certain operating conditions

⇨ Solids require a very complex information structure

Commercial Simulators I

- Commercial simulators can be divided into two groups:
  - equation based systems
    - system is modeled as one large equation system and solved parallel for all variables
      - DIVA, gProms, SpeedUp, Aspen Custom Modeler
  - sequential modular aproach
    - process is divided into connected logical blocks as in a flowsheet
    - blocks are then solved individually
    - recycles solved by iterative solution of the system
      - ASPEN Plus, Hyprotech HySim

Commercial Simulators II

- Problems of available sequential modular systems:
  - Model quality/quantity
    - generally only a few models available for solids processing
    - models usually have low detail level (short-cut models, empirical correlations)
  - Stream structures supported
    - most simulators originate from liquid/gas process industry
    - concentrated parameters such as temperature, pressure, etc. are supported, plus in some cases simple support for distributed parameters such as PSD, but no secondary dependend attributes

Commercial Simulators III

- Characteristics of equation based simulators
  - High flexibility due to equation based design:
    - almost any model can be implemented as long as equations are given and solver supports type of equations
    - custom parameters can be introduced with ease
  - Input of problem requires knowledge of "programming language" → syntax, conventions, etc.
  - Every single model has to be implemented by including the equations → high effort for a simple problem
  - Equation sets get very large, flowsheeting based simulator is closer to engineers view on process

Requirements for a Simulator

- support of flexible information structure for streams
  (distributed and concentrated parameters, standard and custom parameters)
- allow combination of models for individual equipment and process steps to be combined to complex process flowsheet, no limitation to special processes
- presence of fluids and solid/liquid interactions have to be considered
- ergonomic easy-to-use Graphical User Interface (GUI) to allow engineer to build process following his view (flowsheet focussed)
- extendable model database including model backgrounds (mathematical and engineering), model boundaries (valid operating conditions), etc.
- standardized interfaces (e.g. CAPE-OPEN) to other "liquid/gas simulators"

Simulation of Solids Processes at TUHH

1995-1998 Project „Modellierung komplexer Feststoffprozesse“ (‚Modelling of complex solids processes‘) funded by VW-Stiftung

→ Development of program and information structures,
programming of simulation system SolidSim,
simulation of exemplary industrial processes,
no graphical user interface

1999-2002 Attempts to get funding of follow-up projects

- Proposal in 5th EU framework
- Proposal for a AiF project (TUHH only)
  → request to submit a proposal for a cooperation project
  → search for project partners

2003 Begin of funding of cooperation project „Fließschema-Simulation von Feststoffprozessen“ (‚Flow sheet simulation of solids processes‘) by AiF

- Cooperation of 11 universities
- Advisory committee of industrial partners

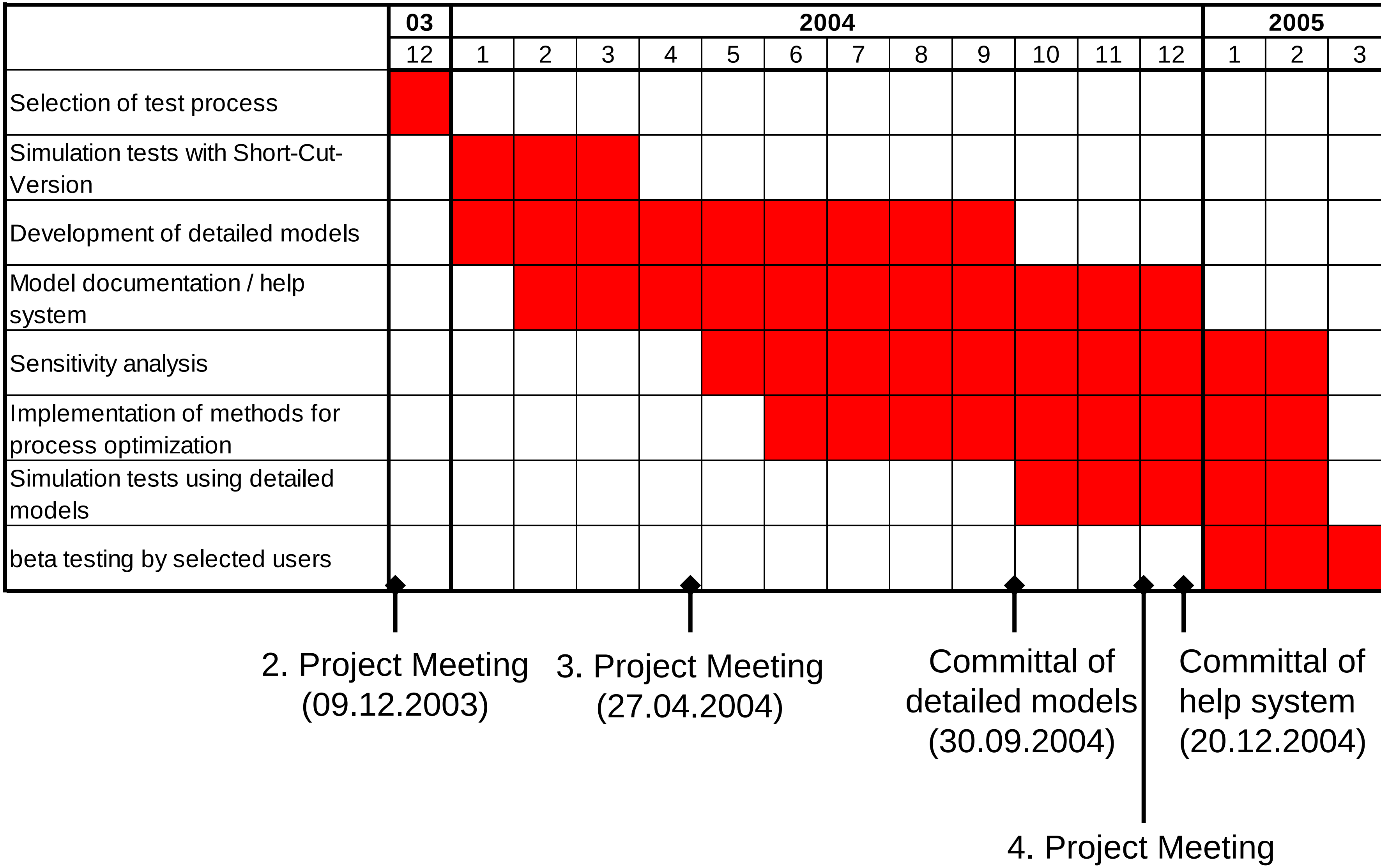
Strategy for Development

- solids processing discipline involves huge number of different process steps and equipment types
- work load can not be handled by one partner
- solids processing discipline is divided into packages and distributed for responsible processing to “most knowledgeable experts” amongst German Universities
- industrial partners of SolidSim project will stand as godfather for each single package
  (both, from industrial users & vendors of related equipment)
- throughout project lifetime there will be several field tests of intermediate results in industry (by industrial partners) to ensure applicability of system and quality of models

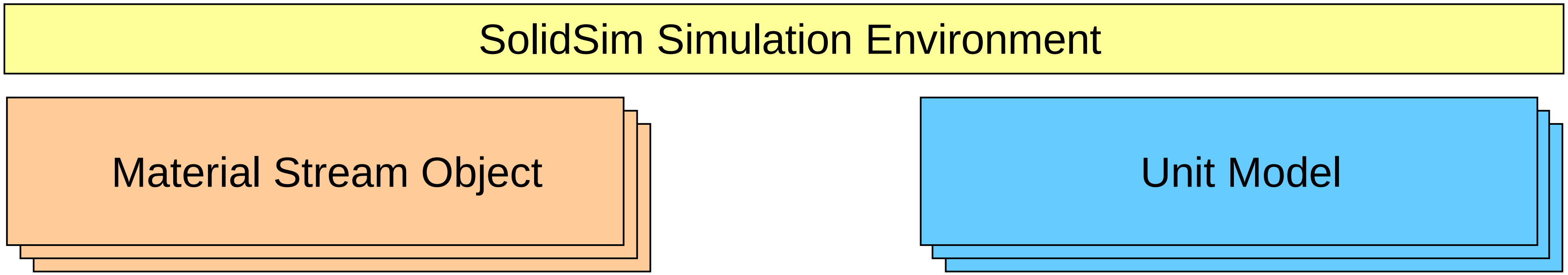
SolidSim Developers

COSE	GUI, Interfaces	G. Gruhn, J. Werther, Hamburg
Size Reduction	Mills	W. Peukert, Erlangen
Solid-Liquid Separation	Filtration Centrifuge / Decanter Hydrocyclone Thickener	S. Ripperger, Dresden W. Stahl, Karlsruhe J. Werther, Hamburg J. Werther, Hamburg
Gas-Solid Separation	Gas cyclone Filter Scrubber Electrostatic Precipitator	J. Werther, Hamburg E. Schmidt, Wuppertal E. Schmidt, Wuppertal E. Schmidt, Wuppertal
Classification	Sifter Sieve Stream classifier	E. Schmidt, Wuppertal J. Werther, Hamburg J. Werther, Hamburg
Agglomeration Granulation	Fluidized Bed Granulator Pressure Agglomerator	L. Mörl, Magdeburg
Drying	Convective Dryer	E. Tsotsas, Magdeburg
Crystallisation Dissolving	Crystallizer	M. Kind, Karlsruhe
Conveying Dossage	dilute phase conveying dense phase conveying Dosage	K.-E. Wirth, Erlangen
Spray	Spray nozzles	P. Walzel, Dortmund
Fluidization	Fluidization	J. Werther, Hamburg

SolidSim Timetable



Design Concept of SolidSim



- Software consists of
  - simulation environment
  - material stream objects
  - unit models

(simulation environment + material stream objects) + base unit → framework

Functions of the SolidSim Framework

SolidSim Simulation Environment

Material Stream Object

Unit Model

- **Providing access to model library**
  - allows for easy development of new models by providing standard programming interfaces and a base module for easy implementation of unit specific models
  - dynamic integration of the unit models into the simulation environment
  - allows to connect individual models to set up a complex flowsheet
- **Graphical user interface**
  - visualization of the flowsheet
  - dialog based user interactions
- **Simulation engine**
  - coordination of flowsheet calculation
  - control of data exchange between unit models and material stream objects during calculation
- **Help system**
  - for simple access to documentation of simulation environment and unit models

Functions of the SolidSim Framework

SolidSim Simulation Environment

Material Stream Object

Unit Model

- **Stream Objects**

  Transports stream information from one unit model to the next

  → Information Stream: Information about process parameter

  → Energy Stream: Information about transferred energy

  → Material Stream: Information about material stream of physical properties
- **Providing access to all stream data necessary for the simulation**
  - Handling of concentrated variables (temperature, pressure) and distributed properties as well (particle size distribution, etc.)
  - Access to physical property package through standardized interfaces
- **Conversion and calculation of derived properties**
  - Example: calculation of thermal velocity distribution out of given particle size distribution and density distribution

Model Library - Guidelines

SolidSim Simulation Environment

Material Stream Object

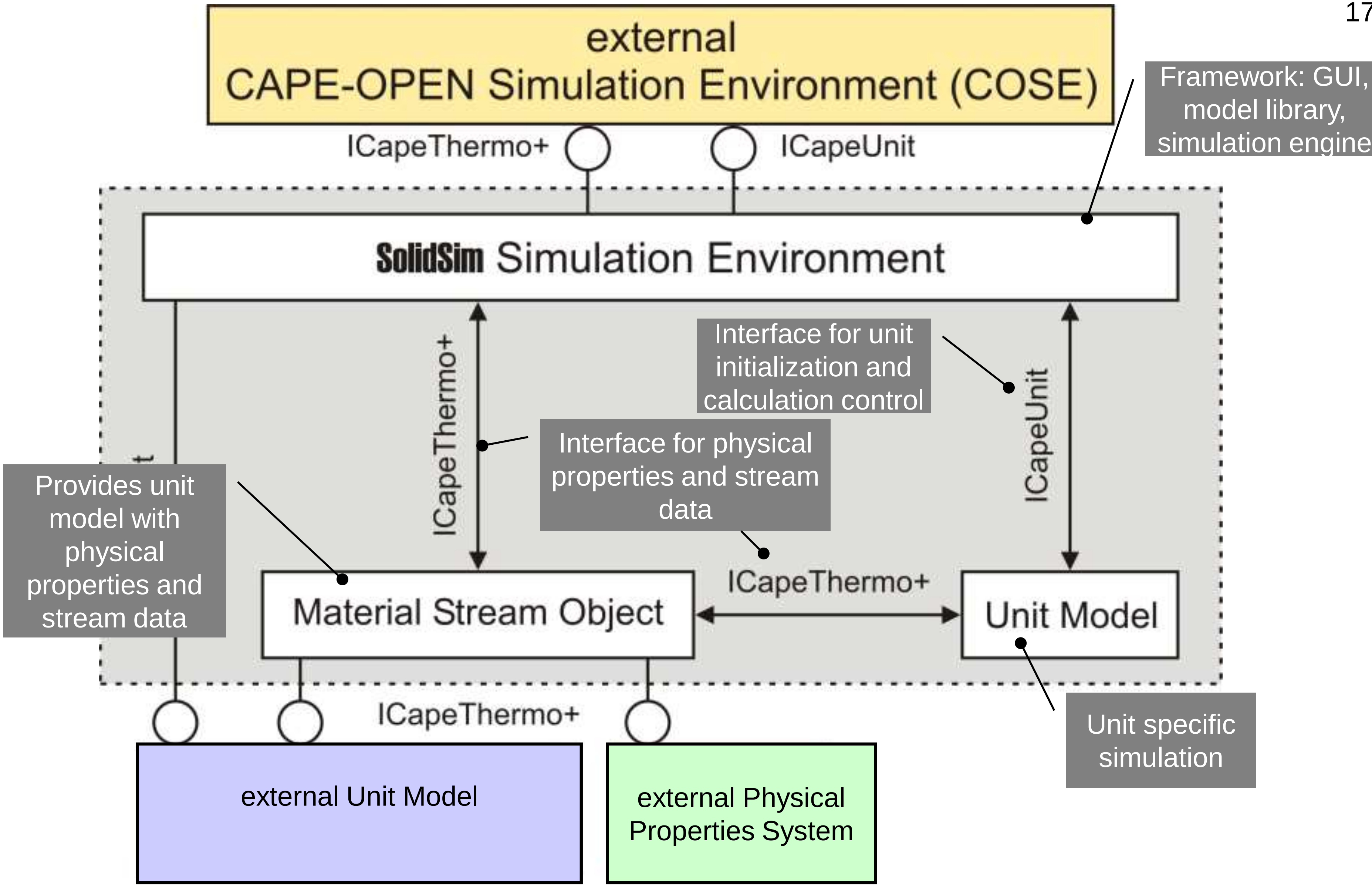
Unit Model

- models will be constantly maintained and supported by experts from University
- models have to be accurately evaluated and tested in industrial applications
- including godfathers from industry ensures practical applicability and relevance
- models have to have good documentation
- models can be replaced by new improved models easily
- new models can be developed and implemented without access to source code of framework

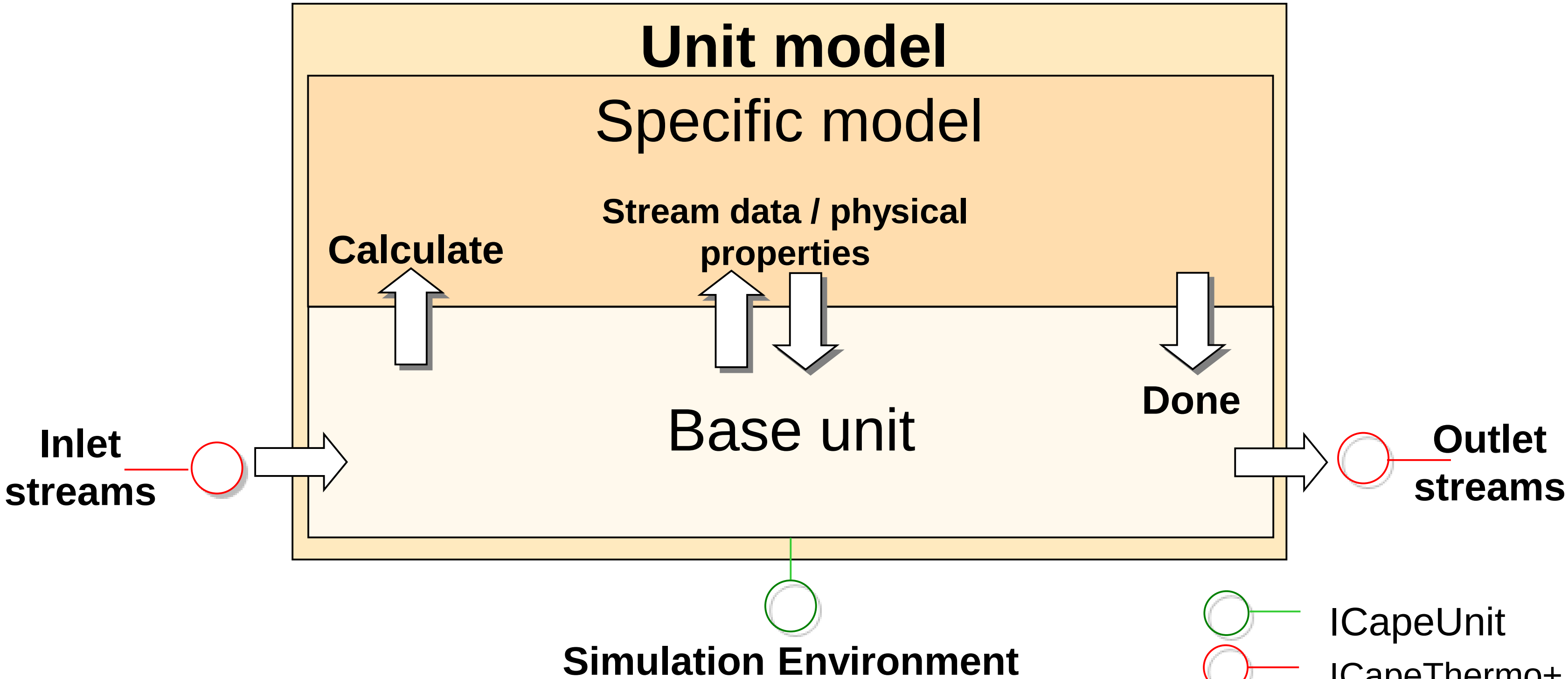
CAPE-OPEN-Standard

- SolidSim utilizes CAPE-OPEN interfaces wherever possible because of the following benefits:
  - Software development
    - shorter development time using existing interface specification
    - Interfaces are validated
  - Interoperability
    - CO compatible units can be used in all COSE‘s
    - One COSE might be used as an unit within an other COSE in a flow sheet
    - Existing solver, physical property packages, databases can easily be used
- With the existing CAPE-OPEN interfaces one cannot handle distributed solids parameters
  - TUHH became an associated member of the CO-LaN in February
  - proposal for the extension of the standard was submitted by TUHH at the end of 2003

SolidSim – Structure of Simulation System



SolidSim – Unit Model



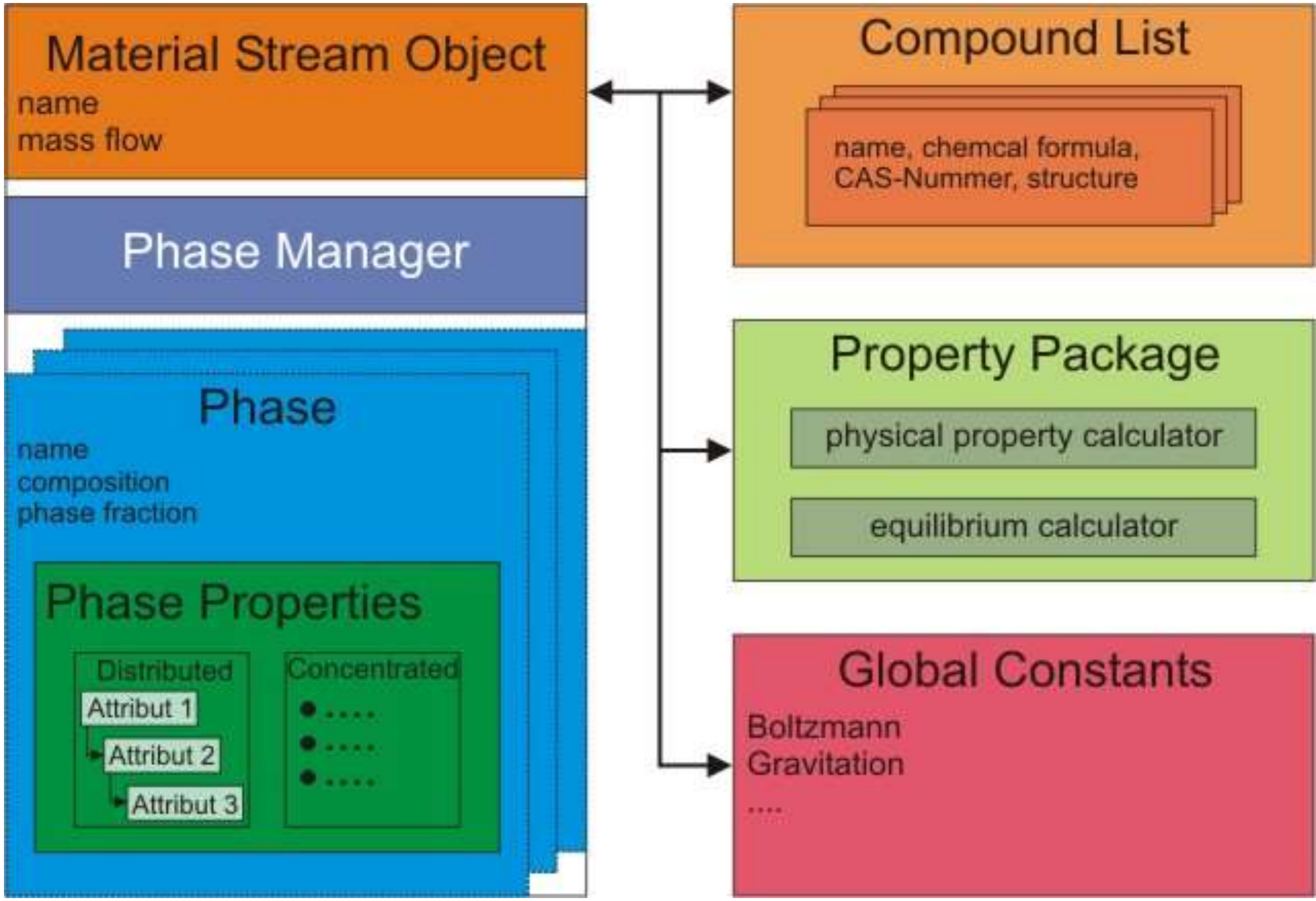
- Base unit provides functionality
  - to simplify communications with stream objects
  - to do standard operations (copying inlet to outlet streams)
  - ensures CAPE-OPEN 0.9.3, 1.0 and 1.1 compatibility
- Specific unit model
  - inherits functionality of the base unit
  - implements unit specific simulation only

→ Unit model developers can concentrate on process simulation

Material Stream Object

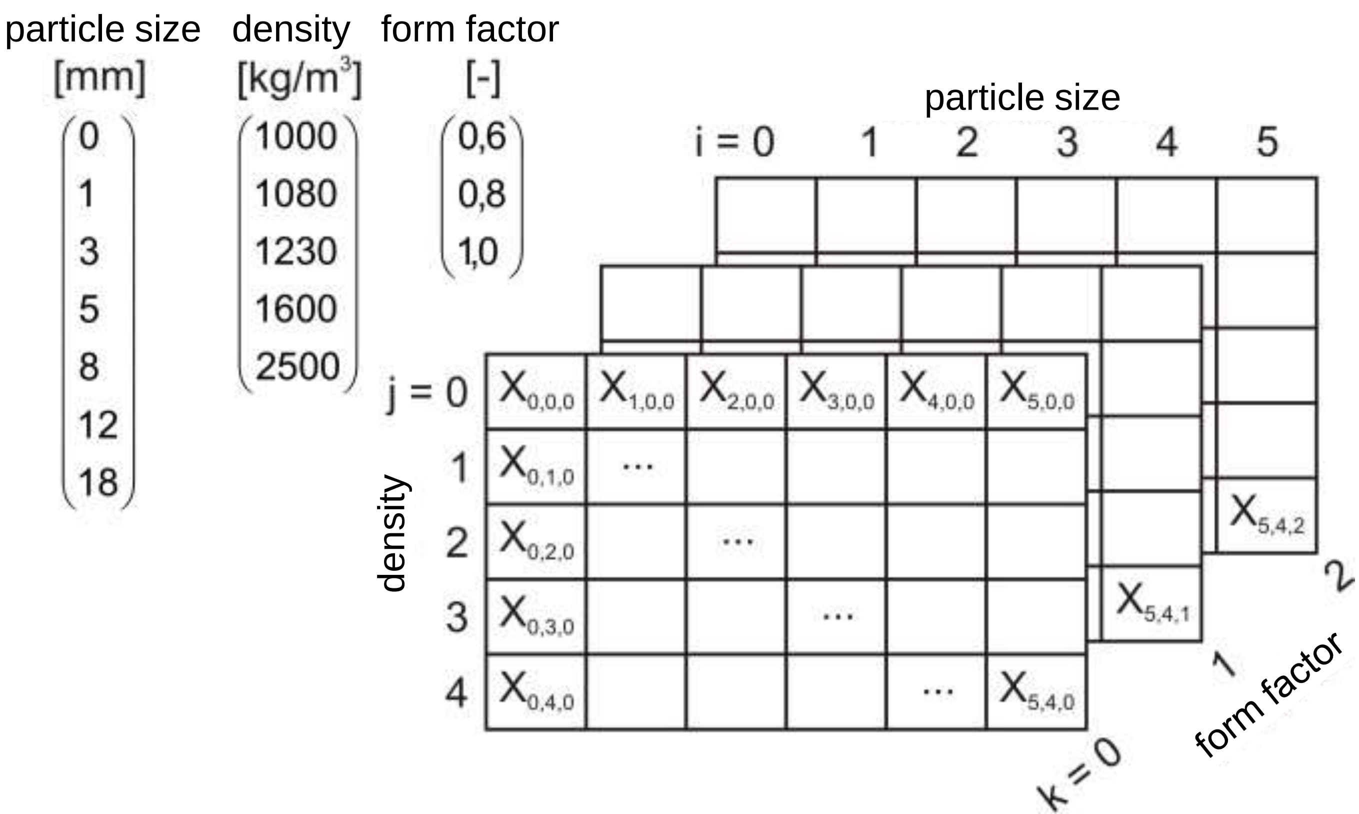
Transports stream information from one unit model to the next and provides access to physical properties

- global definition of all compounds used for simulation
- theoretical unlimited number of phases
  - Phase definition
    - Phase fraction and composition
    - Definition of discrete and distributed properties for each phase
- MO can utilize any CAPE-OPEN compatible physical property package to request physical property or flash calculations
- Access to global constants



Material Stream Object / Distributed Properties

- Distributed properties are stored in a n-dimensional matrix where n is the number of defined properties
- Each element of the matrix is defining the fraction of the particles that can be characterized by a certain combination of properties classes
- The class definition of the distributed properties is stored separately



Material Stream Object / Changing Distributed Properties

- redistribution of mass fractions into existing classes by applying a movement matrix
- entry in movement matrix represents fraction of the material that is moved from the old into the new class
- movement matrix is calculated by the unit model and applies only to the properties the unit requested
- after calculation the unit returns the movement matrix to the framework
- the framework is calculating the new property matrix based on movement matrix

from \ to	1	2	...	n
1	$k_{1,1}$	...	...	$k_{1,n}$
2	$k_{2,1}$	...	...	$k_{2,n}$
...	...	...	...	...
n	$k_{n,1}$	...	...	$k_{n,n}$

Example: movement matrix applied to one distributed property

Extending the Standard

- Extending the existing list of thermo properties
- The functions GetSinglePhaseProp, GetTwoPhaseProp, GetOverallProp will return an interface pointer if a distributed property is requested.
- Adding the following Interface
  - ICapeDistributedProperty
    - GetDistribution
    - GetDistributionState
    - GetDistributionClassDefinition
    - ApplyMovementMatrix

This interface provides functionality to access distributed properties and to change the fractions by applying a movement matrix.

New classes cannot be added.

The initialization of the distributed properties has to be done through a proprietary interface

or

equivalent Set-Functions have to be added to the standard.

CapeOpen 1.1 Thermo Interfaces

<<CAPE-OPEN Interface>>
ICAPEThermoPropertyPackageManager
- +GetPropertyPackageList()
- +GetPropertyPackage()

<<CAPE-OPEN Interface>>
ICAPEThermoPhases
- +GetPhaseList()
- +GetPhaseInfo()
- +GetNumPhases()

<<CAPE-OPEN Interface>>
ICAPEThermoMaterial
- +GetPresentPhases()
- +SetPresentPhases()
- +GetSinglePhaseProp()
- +SetSinglePhaseProp()
- +GetTwoPhaseProp()
- +SetTwoPhaseProp()
- +GetOverallProp()
- +SetOverallProp()
- +ClearAllProps()
- +CreateMaterial()
- +CopyFromMaterial()

<<CAPE-OPEN Interface>>
ICAPEThermoCompounds
- +GetComponentList()
- +GetComponentConstant()
- +GetConstPropList()
- +GetNumComponents()

<<CAPE-OPEN Interface>>
ICAPEThermoContext
- +SetMaterial()

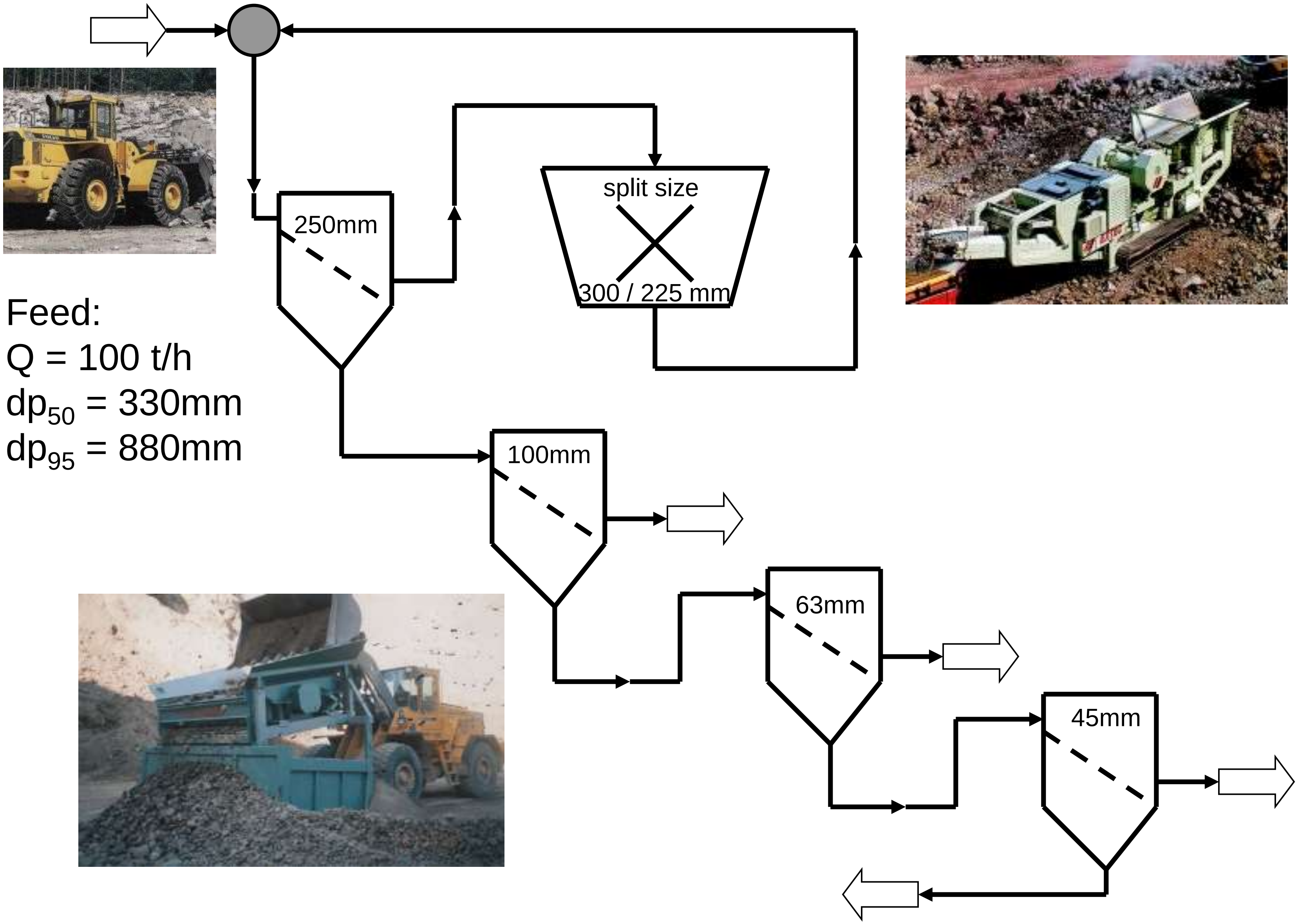
<<CAPE-OPEN Interface>>
ICAPEThermoPropertyRoutine
- +CheckSinglePhasePropSpec()
- +GetSinglePhasePropList()
- +CalcSinglePhaseProp()
- +CheckTwoPhasePropSpec()
- +GetTwoPhasePropList()
- +CalcTwoPhaseProp()

<<CAPE-OPEN Interface>>
ICAPEThermoEquilibriumRoutine
- +CheckEquilibriumSpec()
- +CalcEquilibrium()

<<CAPE-OPEN Interface>>
ICAPEThermoUniversalConstant
- +GetUniversalConstant()
- +GetUniversalConstantList()

ICAPEDistributedProperty
- +GetDistribution()
- +GetDistributionList()
- +GetDistributionState()
- +GetDistributionClassDefinition()
- +ApplyMovementMatrix()
- +SetDistribution()
- +SetDistributionState()
- +SetDistributionClassDefinition()

RWK flow sheet

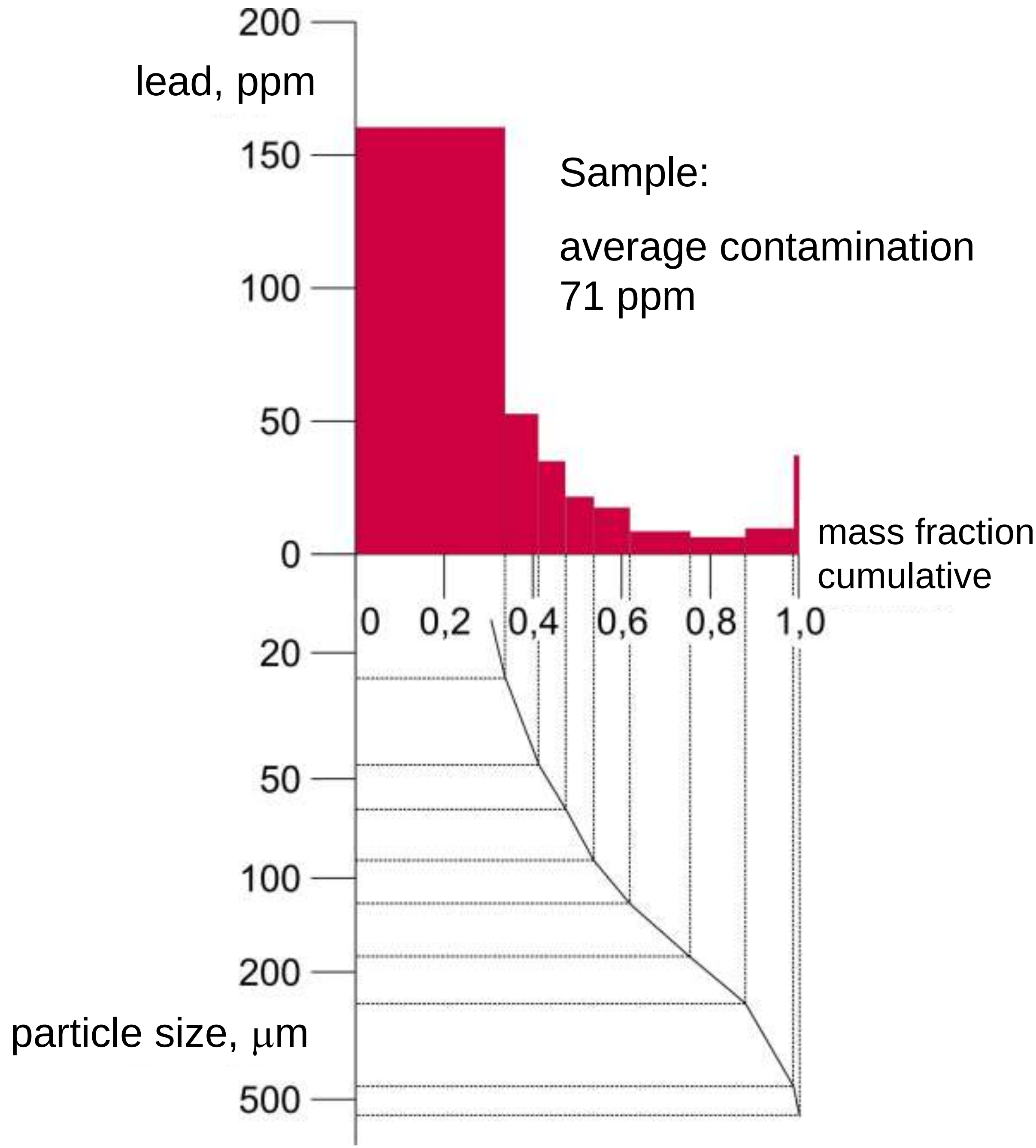


Feed:
Q = 100 t/h
dp_{50} = 330mm
dp_{95} = 880mm

SolidSim
Application:
sewage sludge

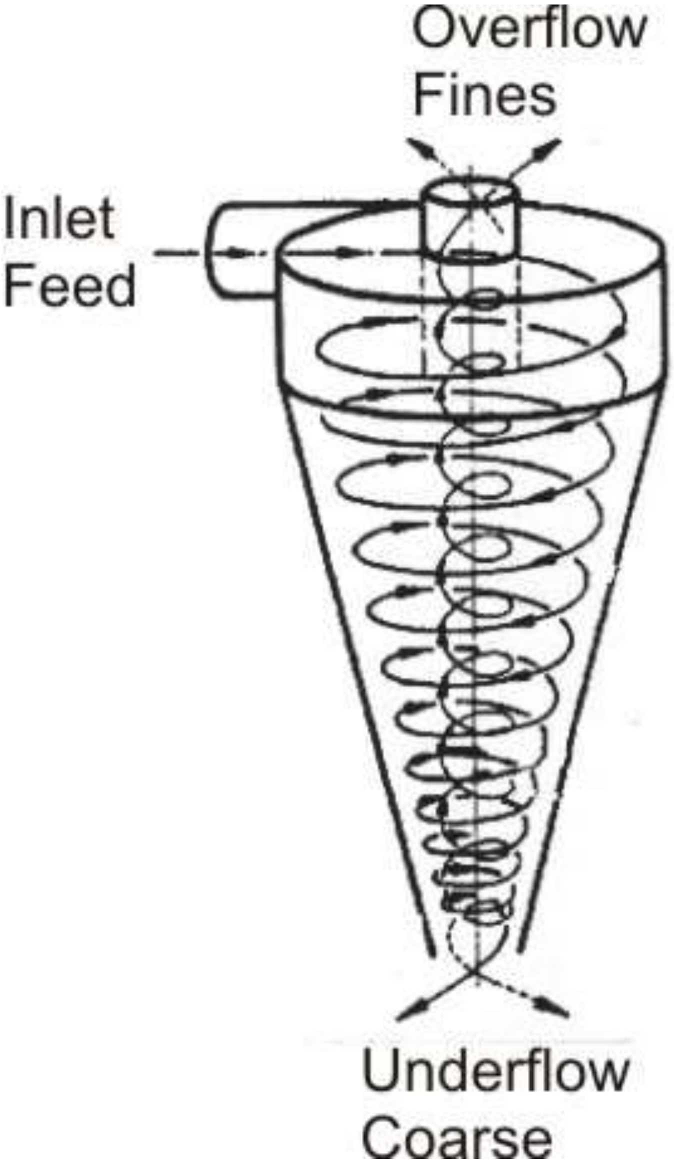
- Problem:
  fine solids are highly contaminated

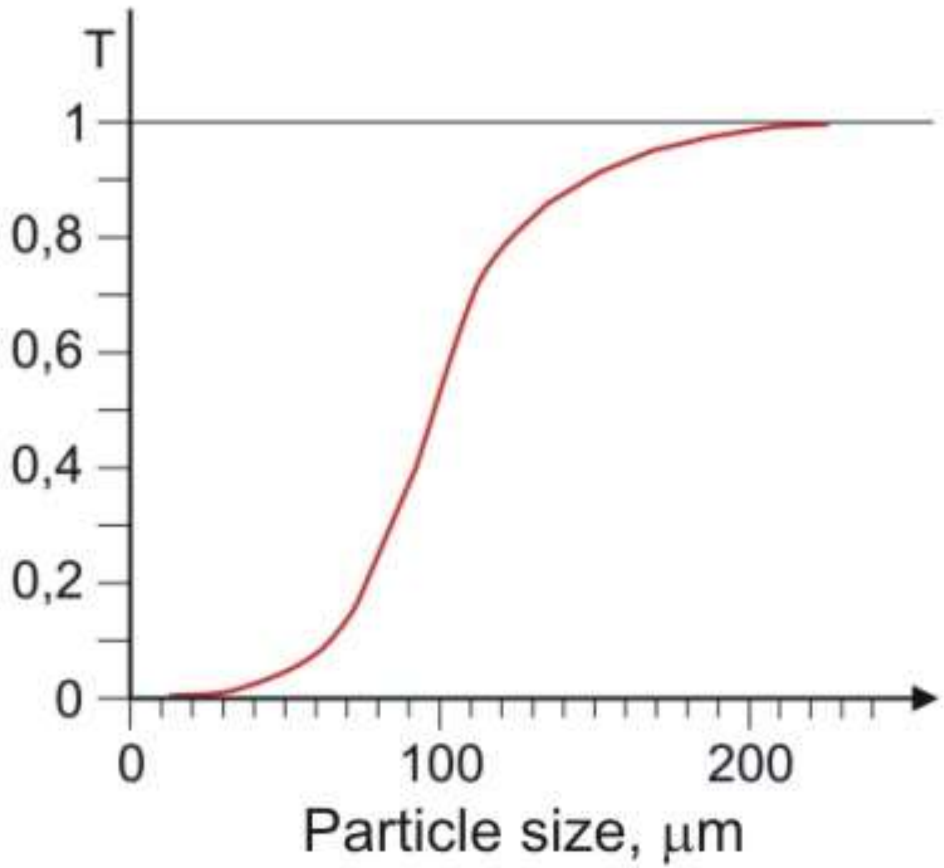
- Solution:
  Separation of the fines in a hydrocyclone cascade



SolidSim

Hydrocyclone – Separation Efficiency





$$T_i = \frac{\text{Mass of size fraction i in underflow}}{\text{Mass of size fraction i in feed}}$$

Thank you for your attention!!

Matthias Pogodda
Denickestr. 15
21073 Hamburg
+49 40 42878-3282