Process Modelling at Purac

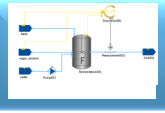
Gerard van Bochove

Advanced Process Modelling Forum 2013
London, 18 April 2013

purac
pure by nature

a csm company

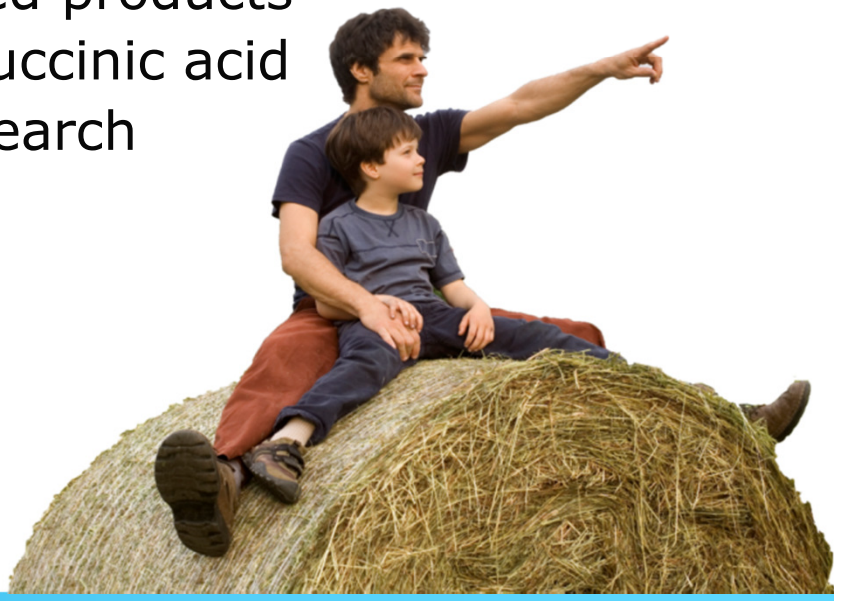
Outline

- Introducing Purac
-  Process modelling at Purac
- Implementation of gPROMS
-  Towards 2014 and further

purac
pure by nature

Purac profile

- Part of Dutch multinational CSM
- Focus on:
  - Natural food preservation
  - Biobased building blocks & chemicals
  - Monomers for bioplastics
- Long history of development, production and marketing of natural lactic acid based chemicals
- Increasing range of bio-based products
- Cooperation with BASF on succinic acid
- 1100 employees, 120 in research



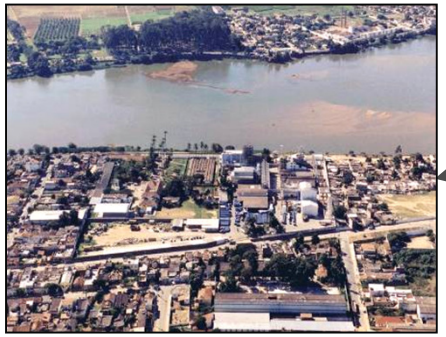
purac
pure by nature

Purac around the globe:

Blair-Nebraska, USA

Gorinchem - Netherlands

PURAC Thailand



Campos – Rio, Brasil

Montmelo, Spain

Map Tha Put, Thailand

Purac's product portfolio

Food market:
- Natural preservation solutions
- Taste & Nutrition solutions

Chemical & Pharma markets:
- Lactic acid, Lactides and Lactic acid derivatives
- Biobased building blocks (Succinic Acid, ..)

Polylactic acid markets:
- L-Lactide monomers for PLA based bioplastics
- D-Lactide monomers for PLA based bioplastics

Medical markets:
- Lactide, glycolide and caprolactone monomers
- Polymers for medical devices and drug delivery

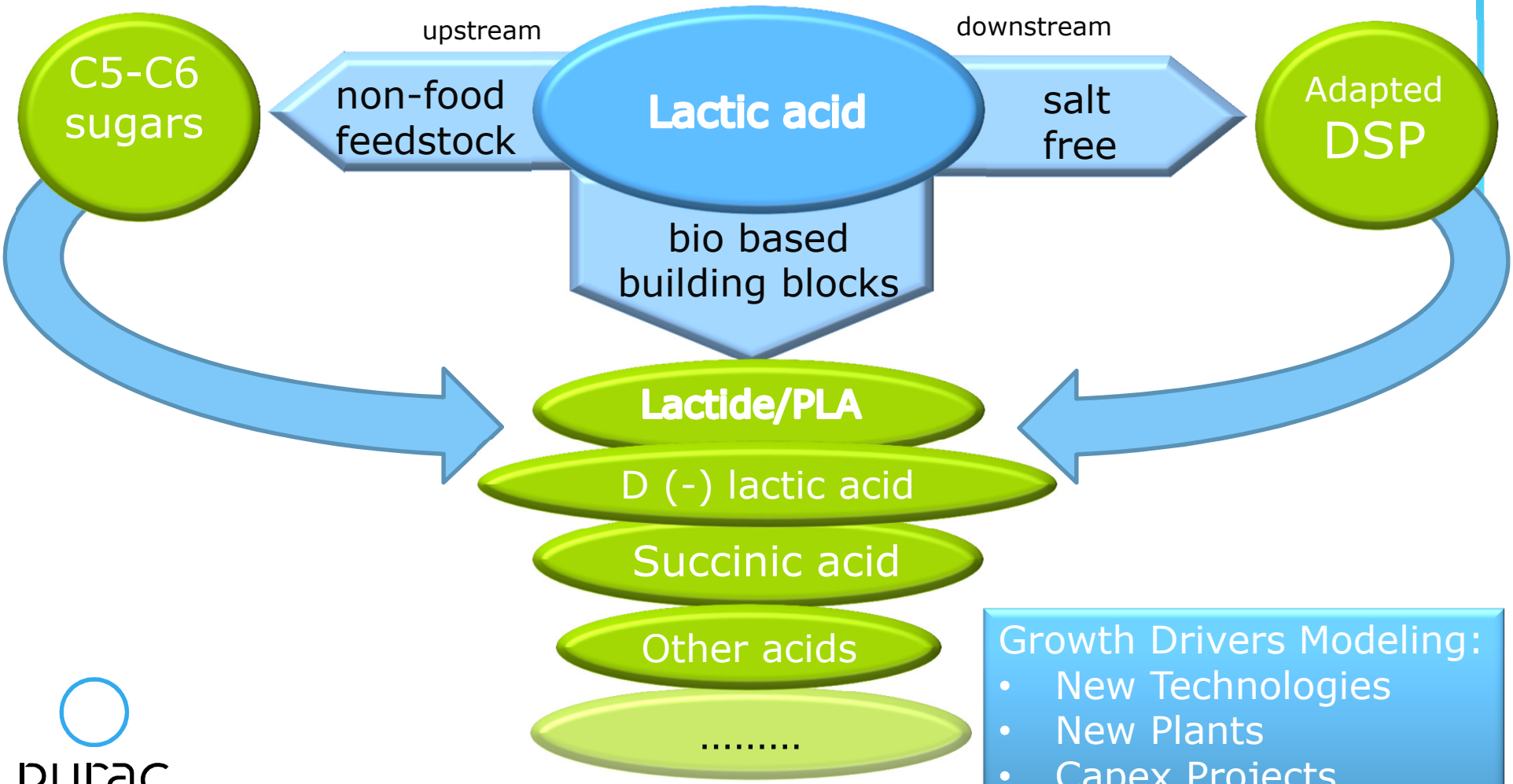
purac
pure by nature

Purac's 'pure by nature' concept

Raw materials from nature	Processes at mild conditions	Products compatible with nature
		
▪ Beet sugar ▪ Cane sugar ▪ Corn starch ▪ Tapioca starch	▪ Fermentation ▪ Crystallization ▪ Filtration ▪ Evaporation	▪ Environmentally friendly ▪ Biodegradable ▪ Low CO_2 footprint

purac
pure by nature

Why we need process modelling…

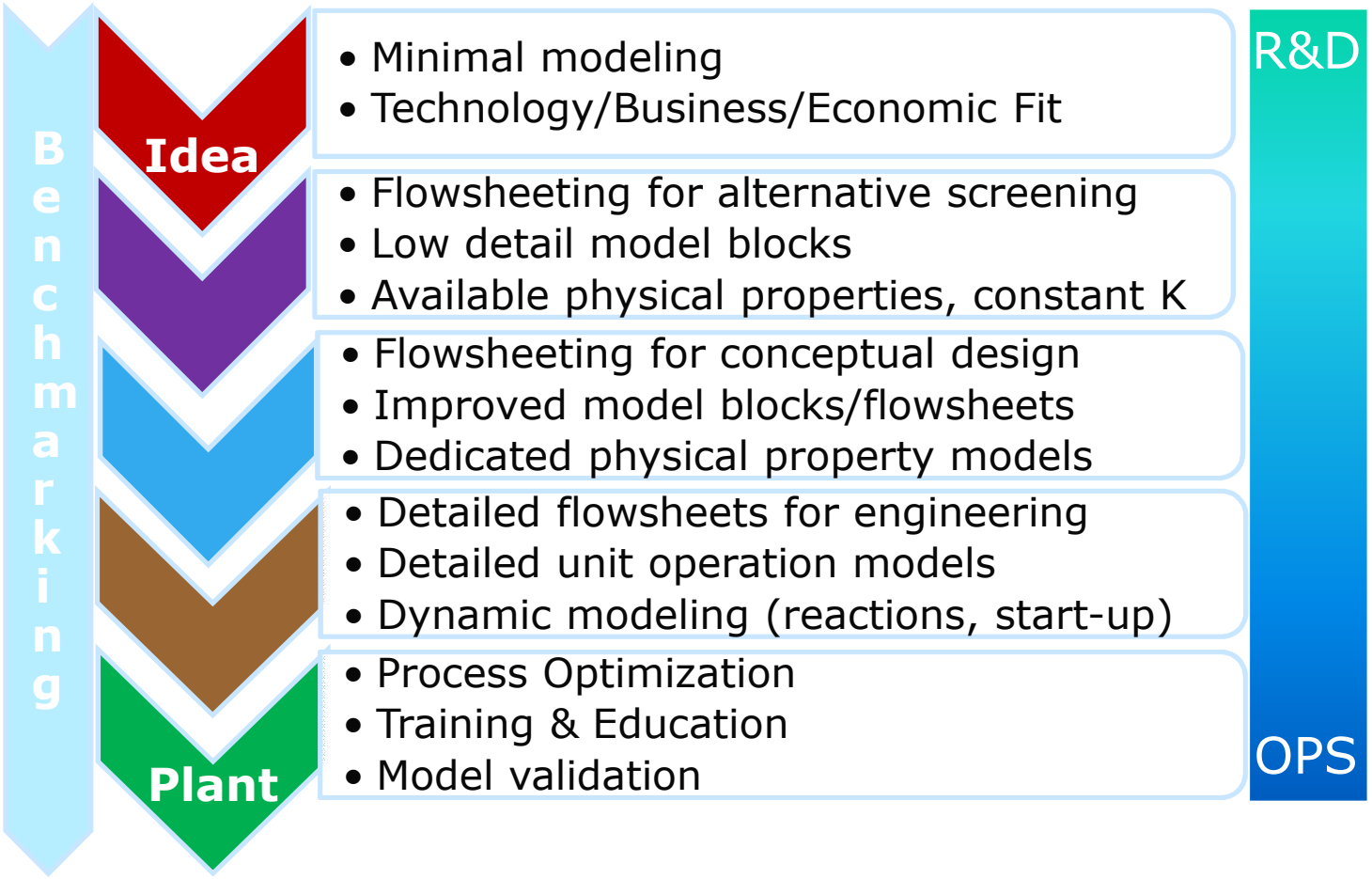


Growth Drivers Modeling:

- New Technologies
- New Plants
- Capex Projects

purac
pure by nature

Place and Scope of Modelling



purac
pure by nature

Why the choice of a modelling platform is not so trivial..

- Products and impurities at Purac are not so common in physical property databases
- Combination of solid, liquid and vapour phases in one process or unit operation
- Unit operations that are less common to chemical industry
- … and covering a wide range: from fermentation to lactide polymerization, from batch to continuous

A platform is needed that allows easy use of

- inhouse databases and model libraries
- steady-state and dynamic simulations
- custom modelling and flowsheeting:

purac
pure by nature

History of gPROMS @ Purac

2006	First evaluation of gPROMS
2006-2008	Dynamic gPROMS model to design lactide synthesis process with complex kinetics and phase equilibria (APMF 2008)
2009-2010	Dynamic gPROMS model for polymerization of lactide to PLA (APMF 2010)
2011	Lactide and PLA plants designed in gPROMS start up successfully!
From 2010	Development of in-house library and in-house physical property databases for flowsheeting. All new R&D projects use gPROMS
From 2012	Engineering uses gPROMS for next generation plants
2013-	Promote use of gPROMS in Operations

purac
pure by nature

Implementation of process modelling

If we want people from R&D to operations to use gPROMS, we need at least to….

- Make sure relevant components, properties and thermodynamics are present
- Provide a model library that
  - Matches with the unit operations present at Purac
  - Contains specific settings and inputs for Purac
  - Has dedicated help and documentation
- Provide training adjusted to specific Purac problems using these libraries and databases
  - *Custom modelling training (R&D)*
  - *Flowsheeting (R&D, Operations)*

purac
pure by nature

Purac Model Library

- Dedicated library of models for Purac's most important **unit operations**, **properties** and **kinetics**
- Collection of unit operation models for detailed modelling or flowsheeting:
  - Wide range of models: Fermentation, oligomerisation, evaporation, polymerization, crystallization, COD-/pH, recycle breaker, etc
  - Different levels of detail or operation modes
- Easy to use for non-experts in gPROMS
  - Dialogue boxes offer selection of predefined settings and properties
  - Provided with links to documentation and starting-values
  - Ready for drag-and-drop flowsheet modeling
- Starting point for model development by experts

purac
pure by nature

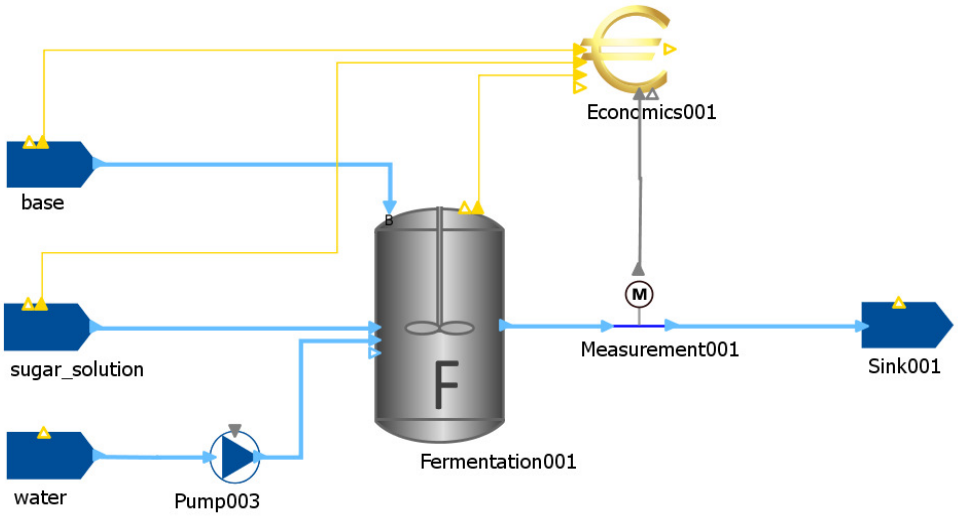
Purac Model Library (Features)

- Provides framework for cost calculations and economic optimization
  - Cost of consumptions and waste streams
  - Utility calculation in unit operation models
  - Calculations for sizing of equipment
- Export of stream reports to Excel
  - *Our wish: Better stream tables with labels in Modelbuilder*
- Separate component list for solid components
  - Excluded from flash calculations
  - Facilitating solid-liquid separating unit operations
- Predefined solubilities for a number of components
  - Planned for this year: electrolyte chemistry

purac
pure by nature

Example: Fermentation

- Two versions:
  1. Steady-state flowsheeting, less detail but with economy
  2. Dynamic, standalone with Excel interface, high detail
- Includes:
  1. Formation of product e.g. lactic acid, succinic acid;
  2. Formation of impurities/ by-products e.g. biomass
  3. Neutralization of organic acids if applicable
  4. Other reactions, checks on solubilities

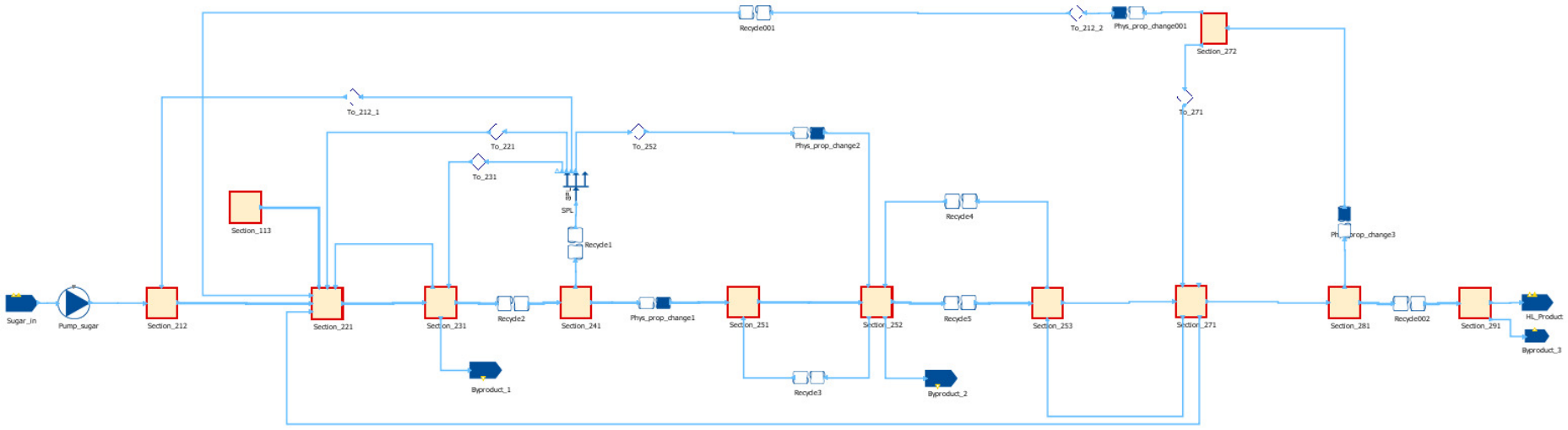


Features:

- *Predefined sets of inputs for different fermentations*
- *Calculates consumptions*
  - *Agitation (electricity)*
  - *Temperature profile (energy)*
  - *Nutrients (costs)*
- *Links to intranet documents*

Complex flowsheets

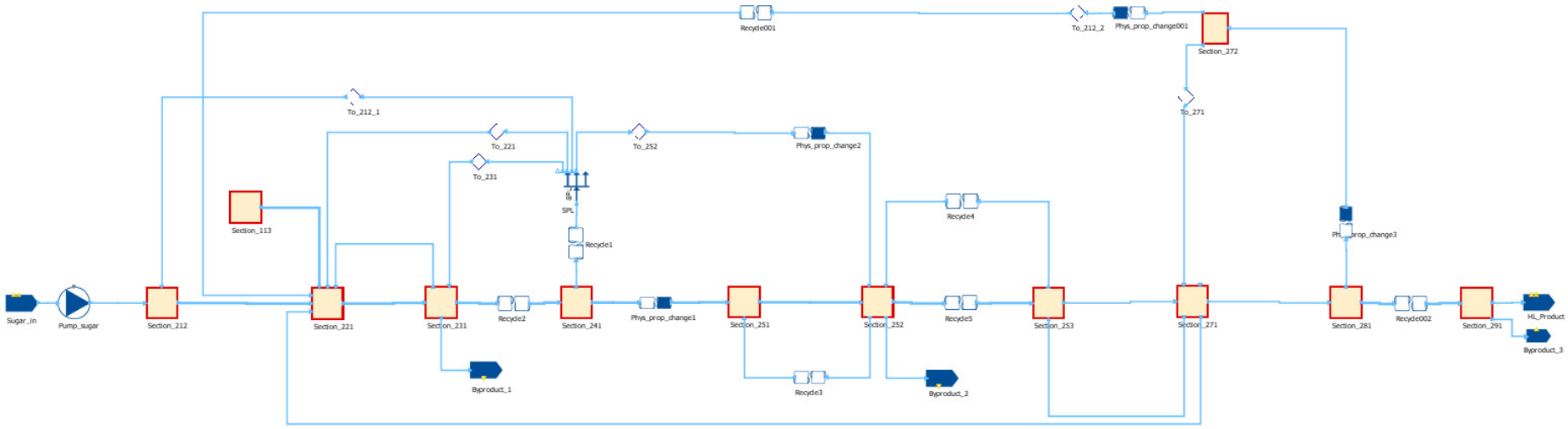
- Biggest challenge: getting a robust and fast converging model that is easy to use
- Library uses dynamics to close recycles and set difficult specifications
- Use of multiple component lists/property sets
- Flowsheet model can be run per section



Example Flowsheet modelling

End 2012/early 2013 existing lactic acid plant model was converted to gPROMS

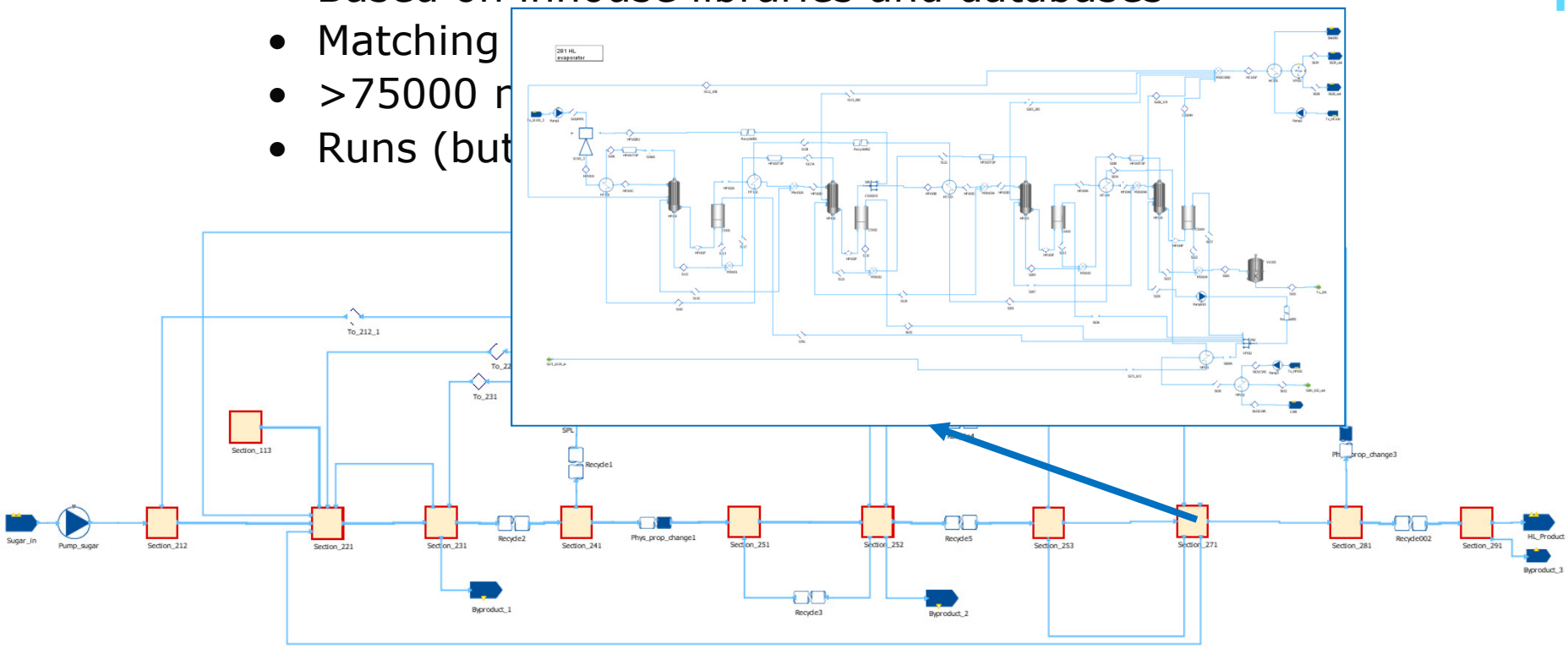
- Together with PSE consultancy
- Based on inhouse libraries and databases
- Matching PFD's
- >75000 model equations, >150000 variables
- Runs (but speed needs to be improved)



Example Flowsheet modelling

End 2012/early 2013 existing lactic acid plant model was converted to gPROMS

- Together with PSE consultancy
- Based on inhouse libraries and databases
- Matching
- >75000 r
- Runs (but



Implementation of process modelling

If we want people from R&D to operations to use gPROMS, we need at least to….

- Make sure relevant components, properties and thermodynamics are present and correct
- Provide a model library that
  - Matches with the unit operations present at Purac
  - Contains specific settings and inputs for Purac
  - Has dedicated help and documentation
- Provide training adjusted to specific Purac problems using these libraries and databases
  - *Custom modelling training (R&D)*
  - *Flowsheeting (R&D, Operations)*

purac
pure by nature

Physical property packages

- Cape-Open connection to Aspen Properties or another physical property package
  - \+ Easiest to implement
  - \- Too slow, not always robust
- IPPFO (ideal)
  - \- Limited capacity and possibilities
- Multiflash
  - \- Limited database, limited visualization
  - \+ Most integrated of all existing physical property packages
- Own physical property package
  - \+ Maximal fit to needs
  - \- Labour intensive

purac
pure by nature

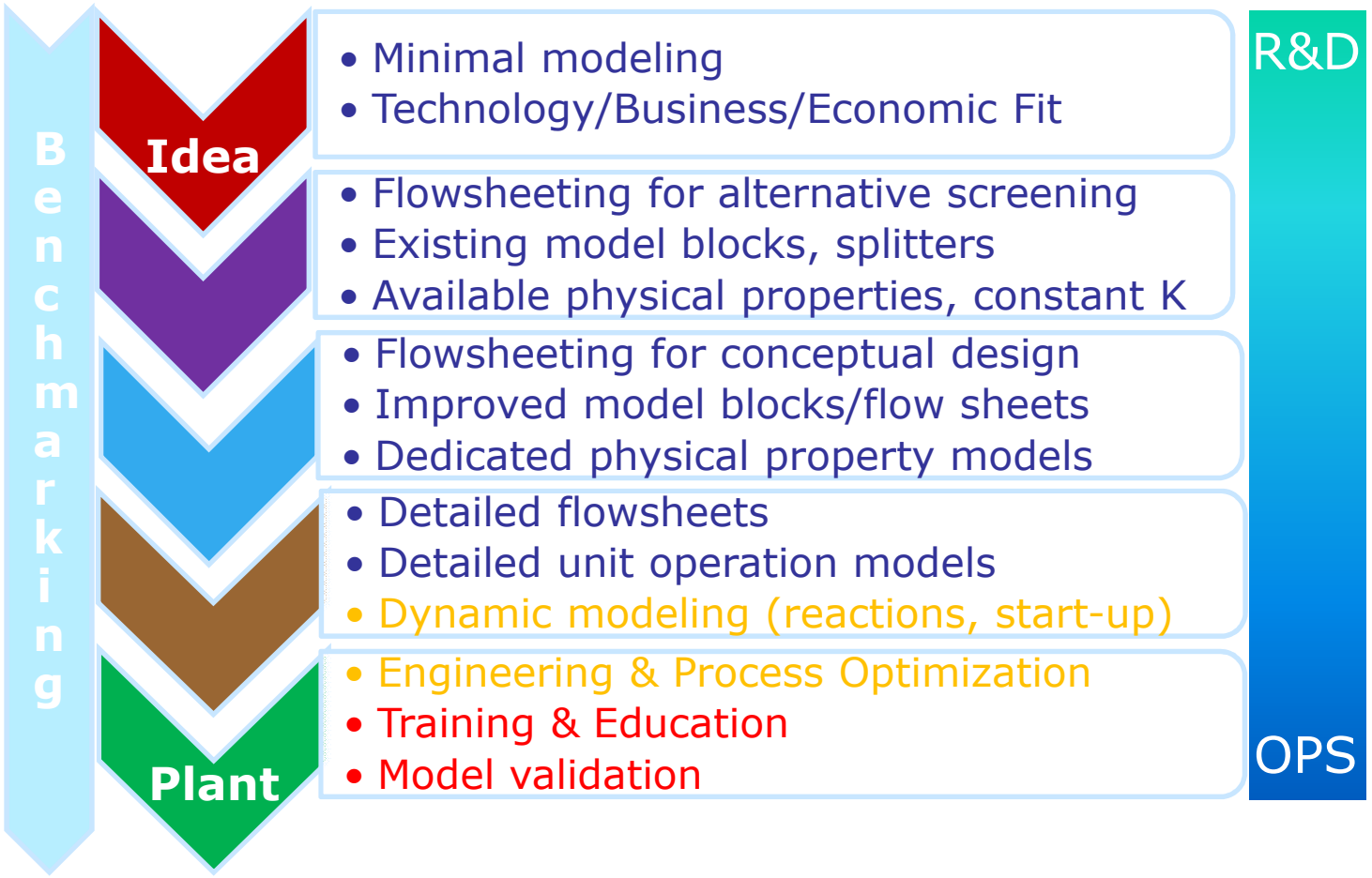
Physical properties: Multiflash

Multiflash:

- Most integrated of all existing physical properties and further integration in gPROMS promised by PSE
- Supposed to give most robust and stable simulation because analytical derivatives are sent to gPROMS
- Possibilities to set up inhouse databases for pure and binary component properties
- Actions that were needed:
  - ✓ Setup inhouse databases for pure components, pseudo components and solid properties and NRTL parameters
  - ✓ Salts added both as solid and as dissolved components to database with different physical properties
  - ✓ Stability issues with strongly nonideal systems with solids present solved with support Infochem and PSE
  - ✓ Excel interfaces to facilitate visualization of physical properties by non-experts

purac
pure by nature

Status of gPROMS implementation



Almost ready!

purac
pure by nature

Recommendations to PSE

- More support, training and documentation on convergence and robustness
- Improve error diagnosis in execution output
  - E.g. physical properties
- Improve user-friendliness for engineering
  - Units
  - Stream tables and labels
- Improve optimization capabilities
  - For example intrinsic tasks should not be ignored by parameter estimation or optimization
- ….

But maybe this has already been dealt with in gPROMS 4…..

purac
pure by nature

Conclusions

- gPROMS can be used from idea fit, conceptual process design, to engineering and optimization
  - … for batch and continuous processes
  - … for custom modelling by experts
- if you invest time in library development and physical property databases
- and involve people from all of the organisation

Purac's strategy aims for many new products, processes and plants:

Process modelling will make the difference!

purac
pure by nature

a csm company