

Process Systems Enterprise and CAPE-OPEN

2nd Annual US CAPE-OPEN meeting
National Energy Technology Laboratory
Morgantown, West Virginia

25 May 2005

Benjamin R. Keeping
gPROMS Kernel and Solvers team leader

- Process Systems Enterprise

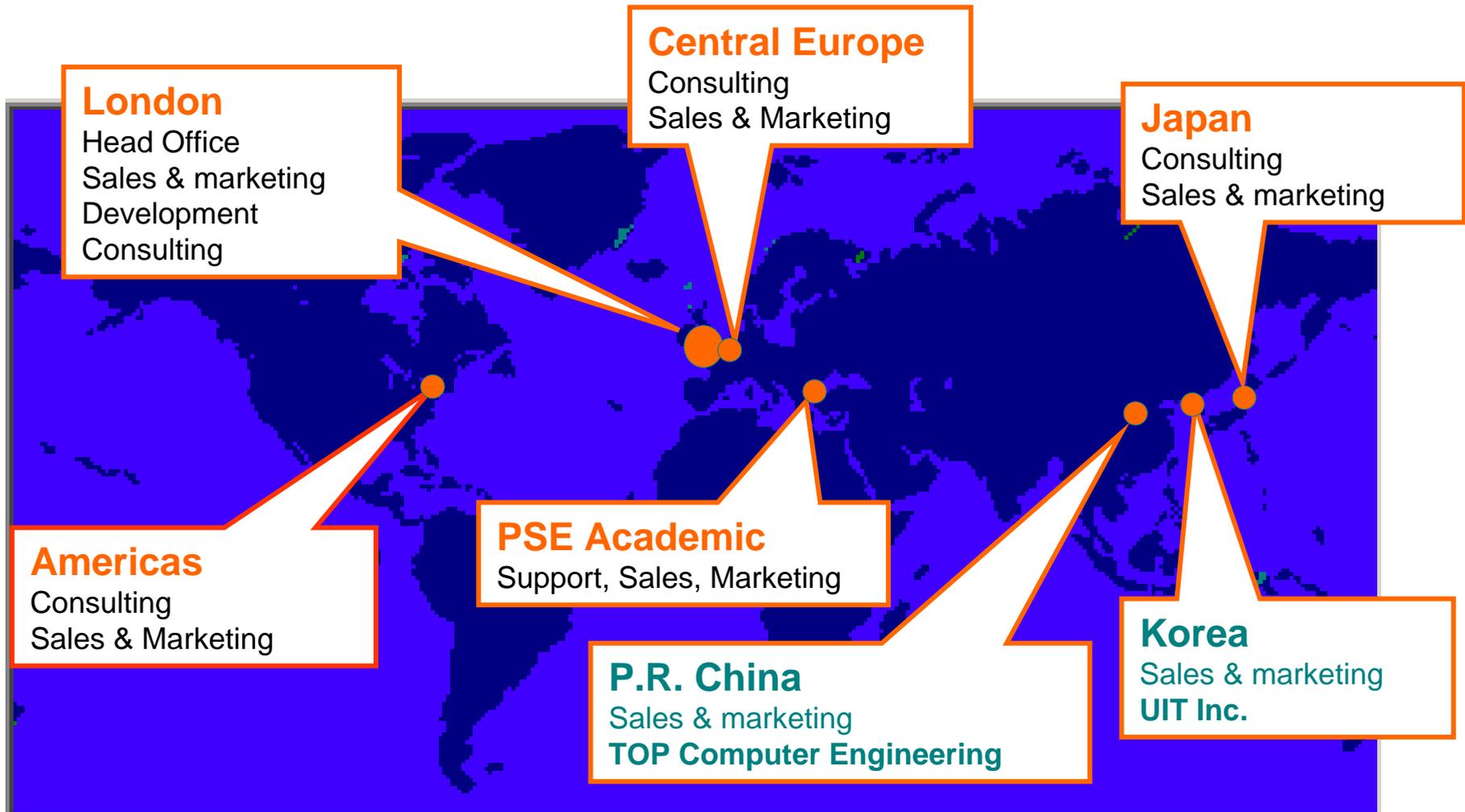
- Products
 - gPROMS®
 - ModelEnterprise®
 - ModelCare®

- gPROMS and CAPE-OPEN

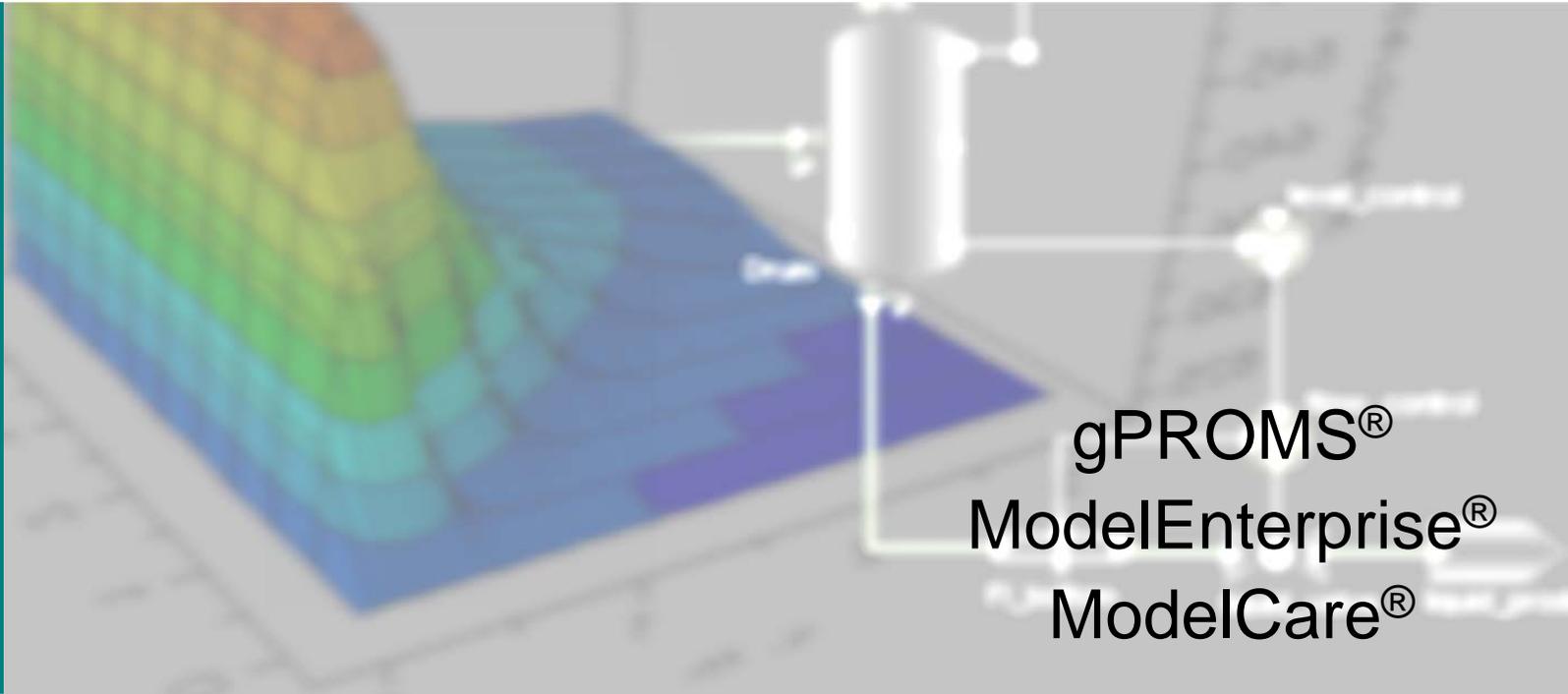
- PSE's perspective on CAPE-OPEN

Help industrial organisations
establish and maintain an
effective modelling infrastructure
for innovation, design and operation
of products and processes

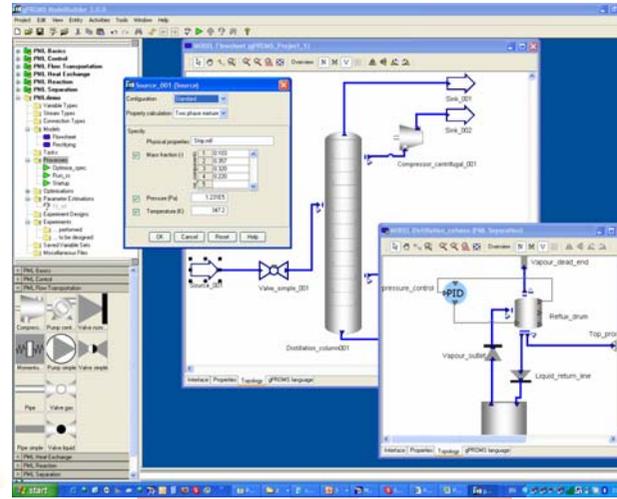
PSE achieves this via a programme of
continuous innovation
in its software & service products



Products

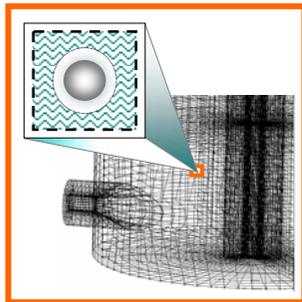


gPROMS ModelBuilder



Fluent® or STAR-CD®
Multi-processor option
for FLUENT®

Options:
optimisation,
parameter estimation,
experiment design



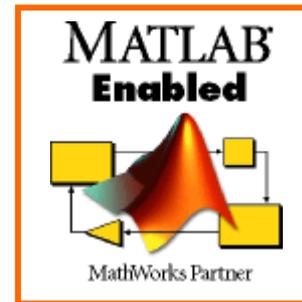
gO:CFD



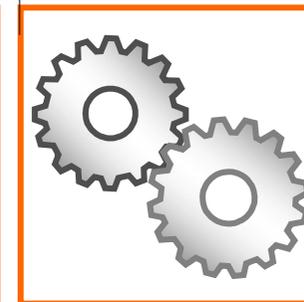
gO:CAPE-OPEN



gO:Simulink



gO:MATLAB

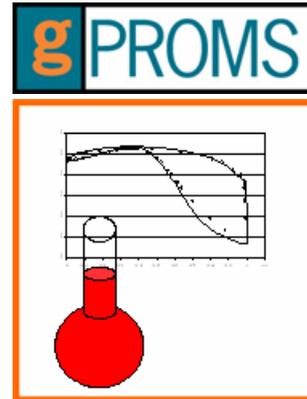


gO:Run

2. General options for modelling tools

■ gPROMS Properties

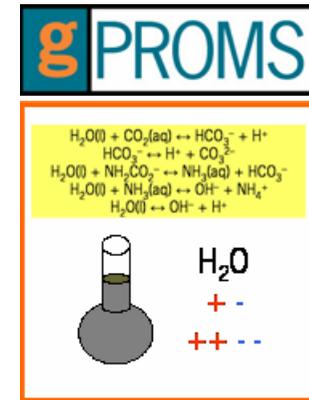
- making use of Multiflash[®] engine
- options:
 - DIPPR databank
 - PC-SAFT model
 - CSM model
 - IAPWS 95 model



gPROMS Properties

■ gPROMS OLI[®]

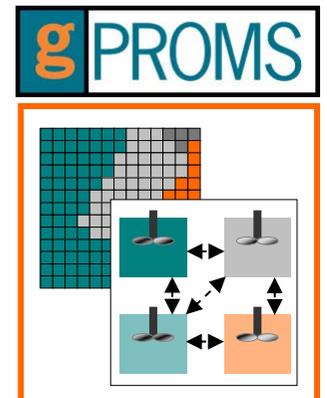
- electrolytic thermodynamics



gPROMS OLI

■ Hybrid Multizonal gPROMS/CFD interface

- available for FLUENT[®]



Hybrid Multizonal

3. Advanced Model Libraries (AMLs)

1. Fixed Bed Catalytic Reactors

- axial, radial and intra-particle variations
- surface chemistry
- bed/wall heat transfer
- optional link to CFD for modelling of shell-side in multitubular arrangements

2. Solution Crystallisation

- nucleation, growth, attrition
- crystal size distribution
- optional hybrid gPROMS multizonal/CFD modelling

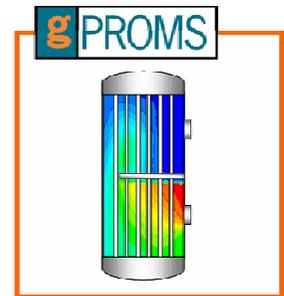
3. Gas-Liquid Contactors

- Maxwell-Stefan formulation
- axial and boundary layer variations
- basic building blocks combined in “flowsheet” to model any column configuration

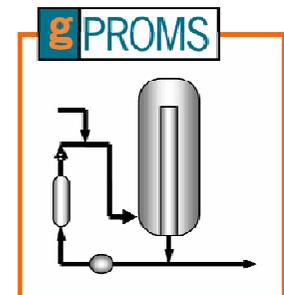
■ Used stand-alone or within complete plant flowsheets

- fully compatible with standard gPROMS Process Model Library

■ Steady-state & dynamic simulation, optimisation, parameter estimation, experiment design



AML:FBCR

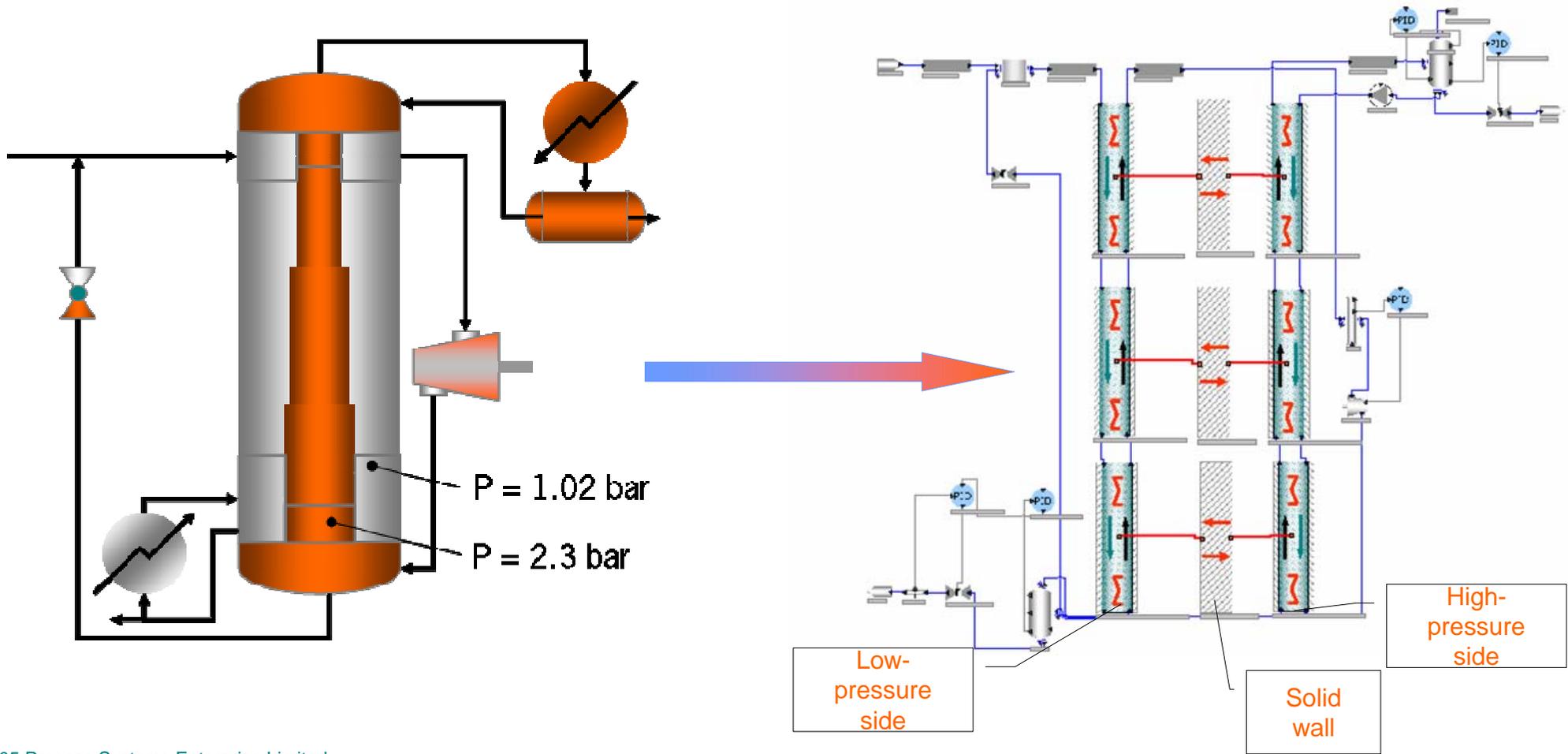


AML:SC



AML:GLC

Example: Heat-Integrated Distillation Column (HIDiC)



4. The gPROMS Engine

Current 3rd-party software applications

- ABB Automation
 - PVC Reaction[®]
 - Dynamic Solutions Flowsheeting[®]
 - Online Simulation
 - Online Estimation
 - Online Optimisation

- FL Smidth Automation: CEMulator[®]

- Honeywell: Shadow Plant[®]

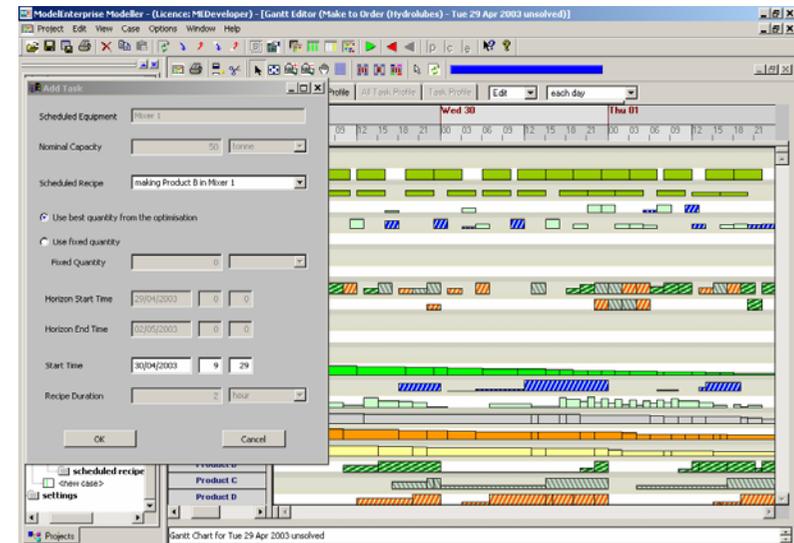
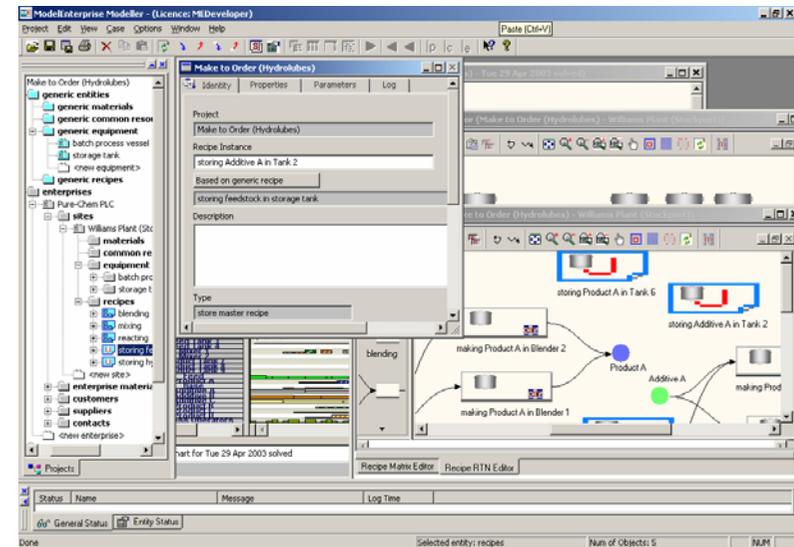
- IPCOS
 - INCA[®]
 - Pathfinder[®]

- Plus...
 - 4 proprietary in-house developments
 - 5 academic developments

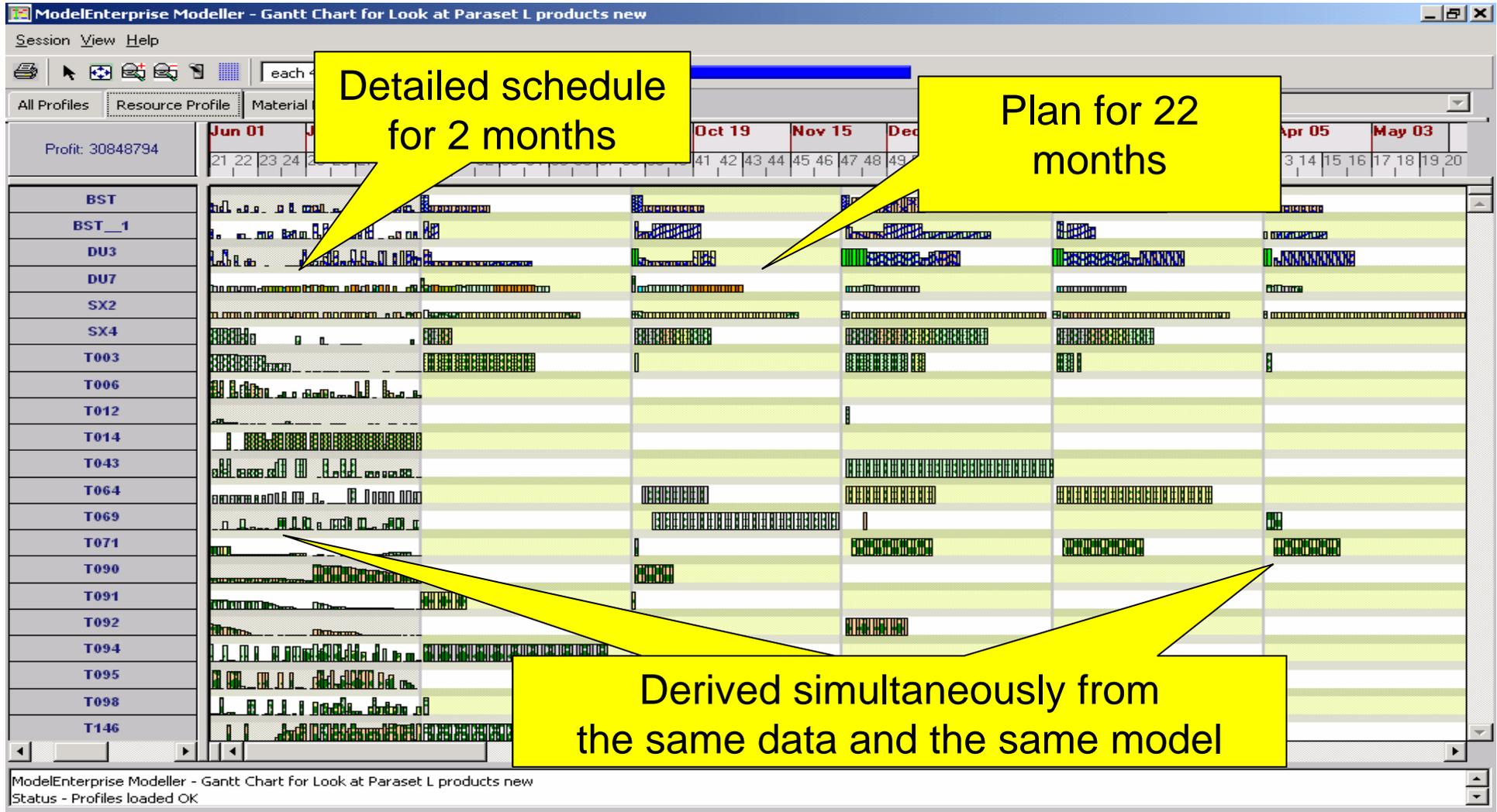
- ...all making use of standard gPROMS-Based Application (gBA) architecture
 - standardised interaction with gPROMS Engine
 - standardised licensing

...an integrated
model-based
platform
to manage
business decisions

for design, planning
and operation of
flexible enterprises



ModelEnterprise Integrated planning/scheduling

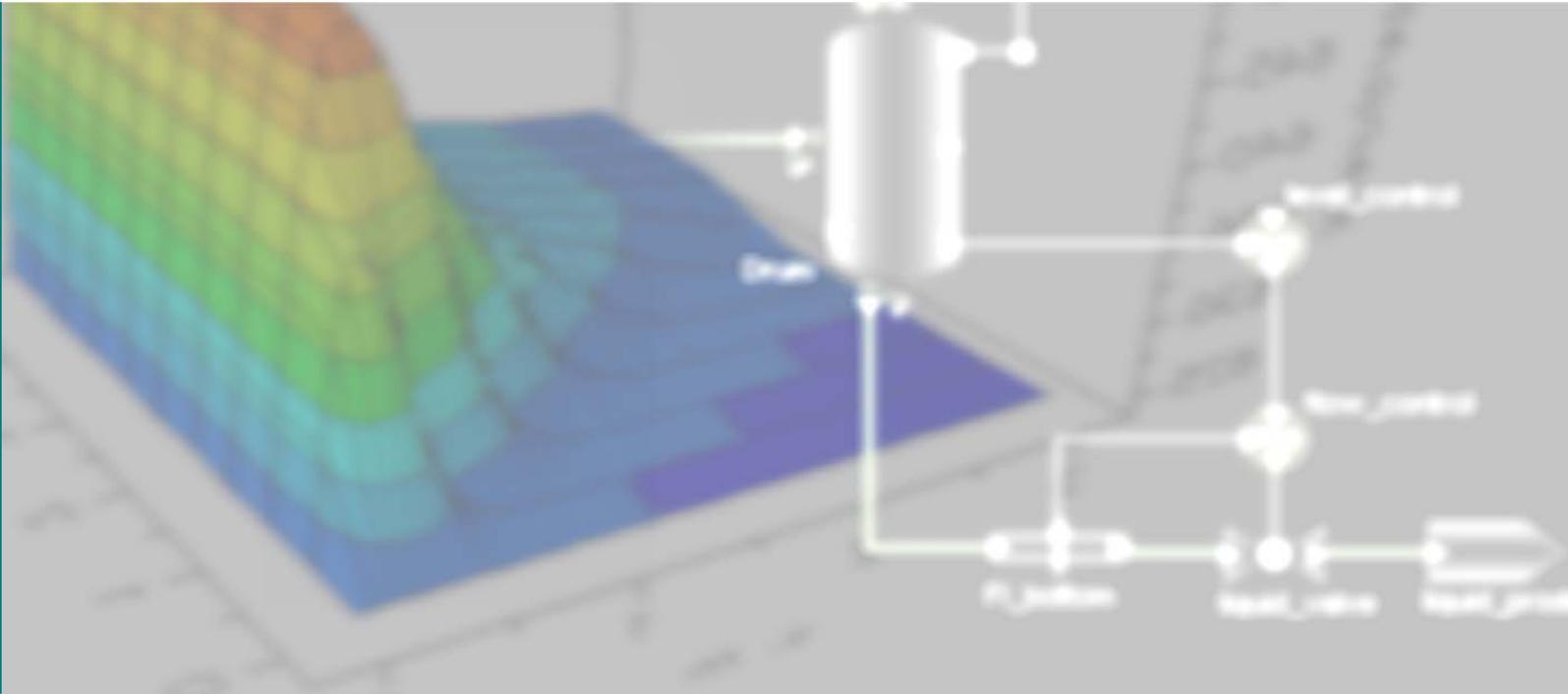


- ModelCare services
 - projects
 - modelling support
 - training
 - superuser mentoring
- Work in close collaboration with customer personnel
 - gain understanding of business objectives
 - guide experimental programme
 - transfer to customer
 - model
 - ability to maintain and extend model
- Aim for fast project turn-around
 - typically 4-6 months



- **Advanced reactors**
 - multitubular (Korea; France)
 - fluidised bed (USA)
- **Crystallisation**
 - chemicals (USA)
 - consumer goods (USA)
 - other (Europe)
- **Advanced separations**
 - membranes (USA)
- **Plant optimisation**
 - new process (Japan)
 - ethylene (USA/Brazil)
- **Plant safety analysis (USA)**
- **New process development**
 - chemicals (Japan)
- **Energy**
 - hydrogen (Japan)
 - power generation (UK)
 - fuel cells (USA; UK)
- **Miscellaneous**
 - oil reservoirs (UK)
 - nitrates (Chile)
 - metallurgical (Australia)
-

gPROMS and CAPE-OPEN



■ Available now

- gO:CAPE-OPEN
 - use gPROMS models as unit objects within CAPE-OPEN compliant PMEs
- CAPE-OPEN Thermo Socket
 - use CAPE-OPEN compliant physical properties within all gPROMS-family products
- *[CAPE-OPEN Equation Set Object]*
- *[CAPE-OPEN Numeric Solvers Sockets]*

■ Under development

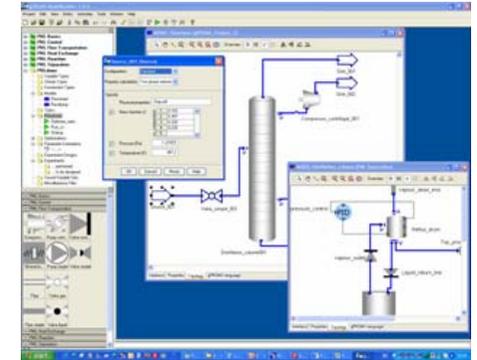
- CAPE-OPEN Unit Socket
- CAPE-OPEN Unit Plug for file-based legacy codes

■ Other interfaces under consideration

PSE's philosophy:

- CAPE-OPEN interfaces must be general
 - cover entire range of gPROMS models and activities
- Benefitting from CO facilities must not require programming in procedural languages
 - accelerate deployment
 - eliminate mistakes
 - maintain transparency and ease of maintenance

- Develop model in gPROMS ModelBuilder
 - ease of model development and long-term maintenance
 - high-level language to describe complex physics
 - Advanced Model Libraries (AMLs) to facilitate model development in specific areas
 - minimisation of time & cost of laboratory experimentation
 - advanced parameter estimation and model-based experiment design
 - use of same model in gPROMS and other environments
 - MATLAB®, Simulink®, Fluent®, STAR-CD®
- Use gO:CAPE-OPEN to deploy model in Aspen Plus®, Hysys®/UniSim®, PRO/II®
 - allow detailed models in plant material & energy balances
 - no need for *a posteriori* adjustments or manual transfer of data
 - still making use of gPROMS advanced solvers

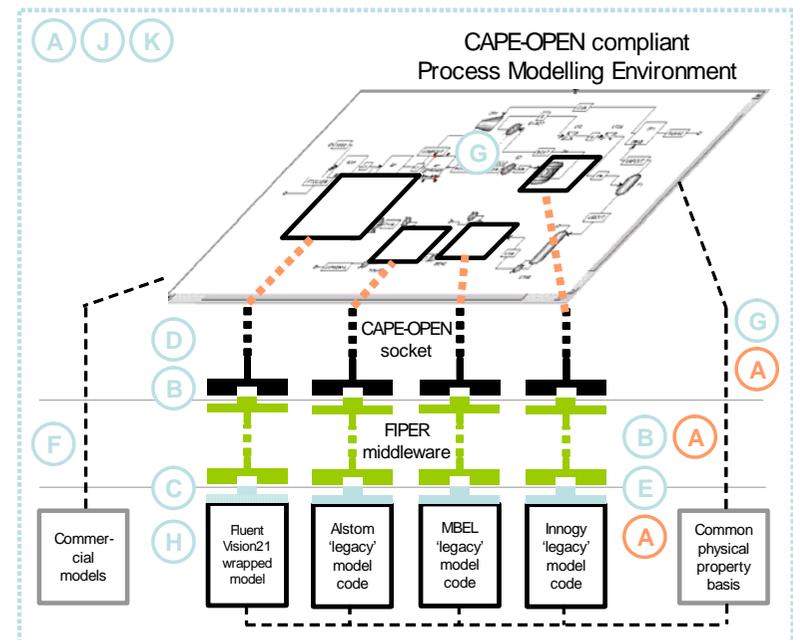


gO:CAPE-OPEN

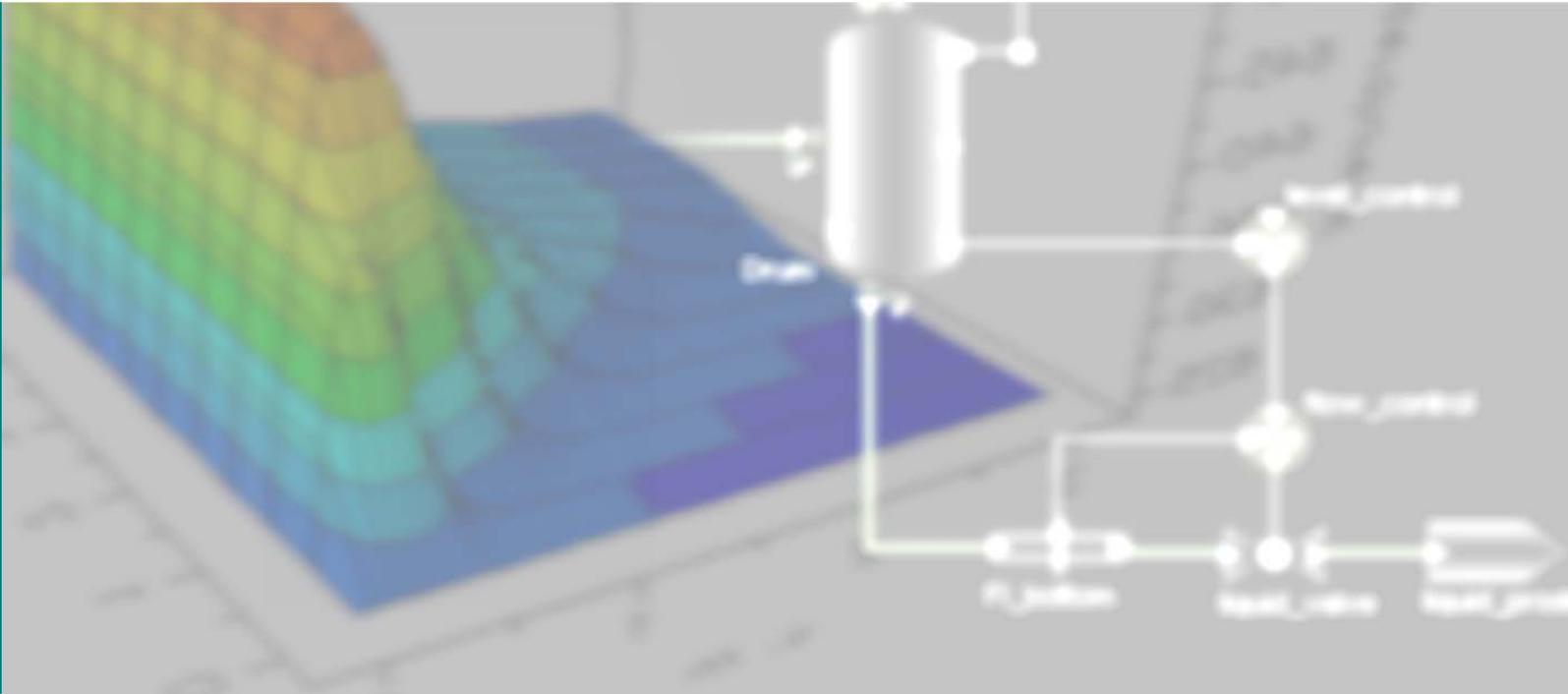
- gPROMS always had open physical properties interface
 - Multiflash[®]
 - IK-CAPE thermo
 - OLI[®]
- CAPE-OPEN standard
 - significantly widens choice
 - ensures consistency between gPROMS models used stand-alone or embedded within CAPE-OPEN PMEs
- CAPE-OPEN Thermo Socket included as standard
 - can be used in all gPROMS-family products
 - gPROMS ModelBuilder, gO:Simulink, gO:MATLAB,
 - complete implementation available in gPROMS v2.3.5

- Allows CAPE-OPEN Unit Objects to be incorporated in gPROMS models
 - can be used in all gPROMS-family products
 - will be made available as standard

- Being developed in context of **Virtual Plant Demonstration Model (VPDM)** project
 - collaborative R&D project in the United Kingdom
 - focus on the power industry
 - supported by the UK Department of Trade & Industry



PSE's perspective on CAPE-OPEN



1. We strongly believe that CAPE-OPEN has brought significant benefits to process engineering software
2. Our experience indicates thermo and (sequential modular) Unit interfaces are at a very good state of development
 - both the standards themselves and the various implementations that are currently available or at an advanced stage of development
3. New standard for modular dynamic unit operations looks promising
 - adoption by “mainstream” modular dynamic simulation packages ?
4. Further progress will need finalisation of standards relating to Equation Oriented technology
 - Equation Set Object
 - Numerical Solvers
 - Equation Oriented Unit Object