ATOFINA example

Making use of CAPE-OPEN interoperability power without developing a CAPE-OPEN interface

Outline

Rate-based modelling of absorption columns

- Software tool used currently presented limitations
- Decision to study the acquisition of a new tool
- Required features of such a new tool
- Solution adopted within gPROMS

Introduction

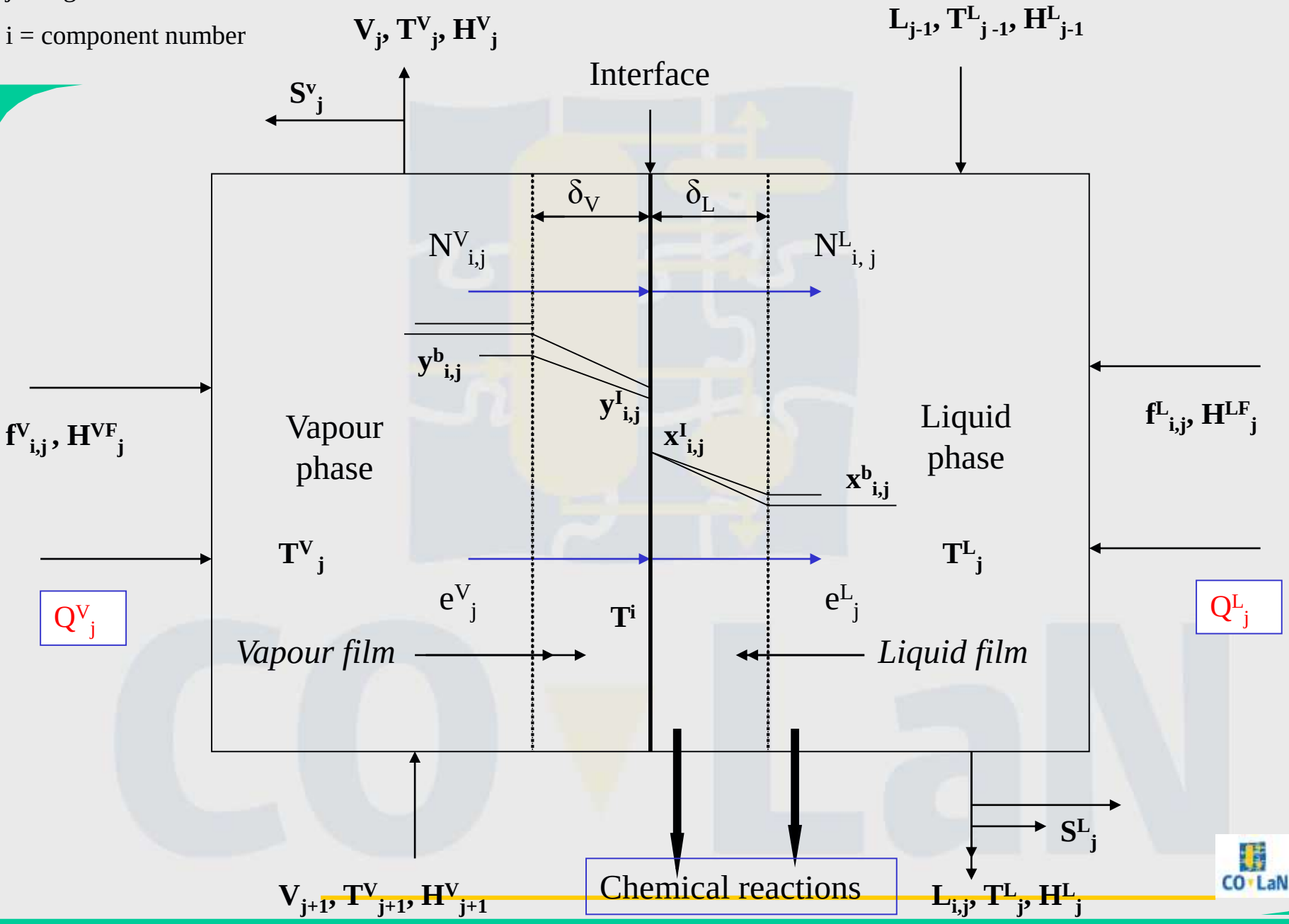
- **Weaknesses of an equilibrium model for absorption**
  - **Main feature: *thermodynamic* EQUILIBRIUM between streams leaving each stage**
  - **Main weakness: in reality DEPARTURE from equilibrium**
  - **Solution adopted: concept of efficiencies**
- **Main drawbacks of equilibrium model:**
  - **Different definitions of efficiencies**
  - **Vapour phase efficiency different from liquid phase efficiency**
  - **Efficiency function of chemical compounds and trays**
  - **HETP function of column height**
  - **Determination of efficiencies or HETP from past experiences: problem with new processes**

Rate-based modelling

- **Main features**
  - Separate balance equations written for each phase
  - Mass and heat transfer rates included in balance equations
  - Separation achieved depends on mass transfer rate
  - Use of the double film theory: equilibrium at interface
- **Main drawbacks**
  - Need of information on the column configuration
  - Use of correlations: possible doubts in their reliability
  - Difficulty of numerical resolution
  - Use of double film hypothesis
- **Main advantages**
  - No concept of efficiencies in the model built
  - Direct calculations of mass and heat transfer

j = segment number

i = component number



Model core

Expression of mass flux: Maxwell-Stefan equation in case of ideal liquid mixture

$$\frac{x_i}{RT}\frac{d\mu_i}{dz} = \sum_{k=1}^{n}\frac{\left(x_i N_k - x_k N_i\right)}{c\text{Đ}_{i,k}}$$

Mole fraction of component i

Molar flux of component i ($mol.m^{-2}.s^{-1}$)

$$\frac{dx_i}{dz} = \sum_{k=1}^{n}\frac{\left(x_i N_k - x_k N_i\right)}{c\text{Đ}_{i,k}}$$

Distance coordinate in the film (m)

Molar density of fluid mixture ($mol.m^{-3}$)

Diffusion coefficient ($m^2.s^{-1}$)

Solving Maxwell-Stefan equation

- **No reactions in the film or reactions neglected: ANALYTICAL solution of Maxwell-Stefan equation**
- **Reactions in the film (fast reactions)**
  - **Rigorous approach**
    - **NUMERICAL resolution of the set of Maxwell-Stefan equations and continuity equation with chemical term**
    - **Numerical methods for 1st order derivatives**
      - **numerical integration by Gear method**
      - **finite difference approximation**
- **Analytical expression with enhancement factor to take into account effect of reactions on diffusion:**

$$(J_i) = (x^I - x^b) F(k_{i,k}) \underbrace{G(N_i, k_{i,k})}_{\text{Enhancement factor}}$$

$$N_i = J_i + x^b N_t$$

Diffusion flux of component i ($mol.m^{-2}.s^{-1}$)

Limitations of current tool

Limitations

- Frequent convergence problems
  - Tool for specialist only
- Mass coefficient transfer calculation
  - Lack of accuracy of correlations for classical random packing (30% off for global $k_g a$)
  - No correlation for recent packing or modern trays (Ex: Vgrid trays, Cascade Mini Rings)
- Heat coefficient transfer calculation
  - Unable to represent high exothermic phenomena

    Ex: Cl_2 absorption by soda with large Cl_2 flowrate

    Incorrect representation of heat transfer from vapour to liquid greater than 20,000 kcal/h.m^2

    Unreasonable calculated vapour temperature (250°C)

Limitations (cont'd)

- Application range too limited through use of enhancement factor
  - ➲ Model not adapted for:
    - Absorption controlled by kinetics
      - Ex: CO_2 absorption by caustic soda
    - Three phase distillation or absorption
- Software development fully stopped by Oct. 31, 2003 after several years without much development already
- Replacement product available by end 2005

Features of model looked for

Model features (1/4)

- **Convergence capabilities**
  - A powerful numerical solving method
  - A good initialisation procedure

- **Mass and heat transport description**
  - Film theory
  - Exact solution of the Maxwell-Stefan equations

Model features (2/4)

- **Absorption and distillation simulations with a large range of internals**
  - **Accurate binary mass transfer coefficient correlations for each internal including up-to-date trays and packings**
  - **Accurate heat transfer coefficient calculation**

Model features (3/4)

- **Reactive absorption and distillation simulation**
  - **“Slow” reactions: reactions taking place in the bulk**
  - **“Fast” reactions: reaction influence on mass transfer in the film must be taken into account**

$$\frac{\partial \mathrm{N_i}}{\partial z} = \sum_{k=1}^{r} \nu_{i,k} r_k$$ in the film

Model features (4/4)

- **Thermodynamic models**
  - Use of any third-party thermodynamic model through CAPE-OPEN compliant interfaces
- **Electrolyte systems**
  - Effect of the electrostatic potential gradient on the diffusion of the ionic species
- **Ability to use developed model within a full process model**
  - Model seen as a Unit Operation through CAPE-OPEN compliant interfaces

The CAPE-OPEN Standard: What it permits

CAPE-OPEN use case #1

- A physical and thermodynamic properties calculations Process Modelling Component developed by a supplier, can be used the same way within several CO-Process Modelling Environments.

- The user saves the time needed to configure the properties calculations parameters for those environments, and gets consistent results by using the same methods and data.

- This is obtained by wrapping the thermo server with CAPE-OPEN standard interfaces.

CAPE-OPEN use case #2

- A Unit Operation model such as a proprietary chemical reactor model, developed by an operator or a process licensor, can be used the same way in most commercial PMEs without any change, without any recoding or recompiling.

- This is obtained by putting the unit operation model to the Unit Operation standard: introduction in a flowsheet, connection of input-output ports, specification of parameters, validity checking, calculation, publication of results.

Solution adopted within gPROMS

Rate-based model of absorbers

- **Solution adopted**
  - ➲ **gPROMS modeling**
    - **Rigorous handling of Maxwell-Stefan equations**
    - **Appropriate model for fast kinetics in liquid film**

- **Limitations**
  - ➲ **gPROMS requires a thermodynamic server**
    - **OLI linked to gPROMS but OLI not licensed by ATOFINA**

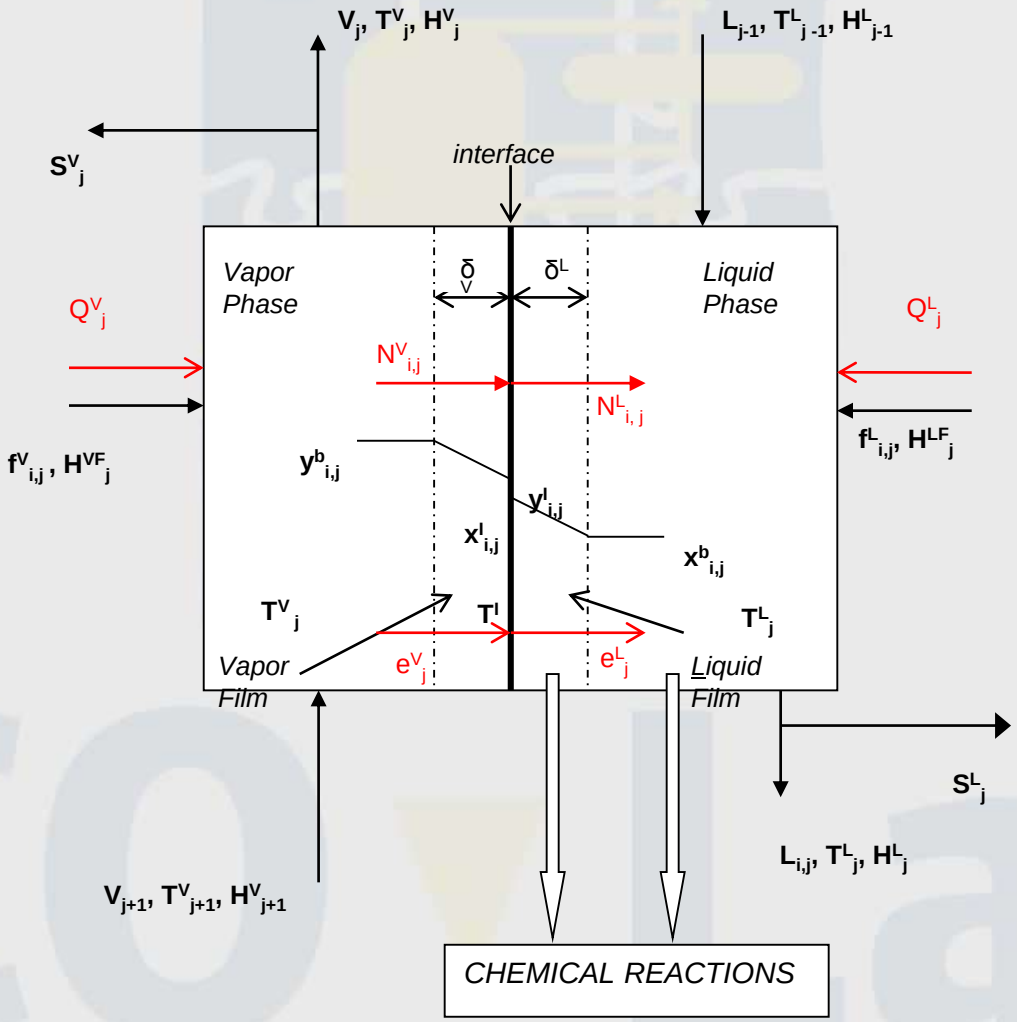
Rate-based model of absorbers

- **User requirements**
  - gPROMS model using an Aspen Plus thermo
    - Typically ELECNRTL
  - gPROMS model used within an Aspen Plus model
    - To be used just as any Ratefrac unit model
- **Technical solutions**
  - Make a CAPE-OPEN Property Package out of Aspen Plus based on ELECNRTL
  - Call this CO PP within gPROMS model through CO Thermodynamics and Physical Properties interfaces
  - Include the gPROMS model as a CO Unit Operation within an Aspen Plus flowsheet

Making a CO Property Package

- Within Aspen Plus
  - Define chemical compounds
  - Define methods to be used for each property
  - Export as a CO Property Package (CO PP)
- Requires Aspen Plus license when being called upon
- Referenced through the name given to the CO PP file
- Registered in the Windows registry as a CO PP within the CO Thermo System supplied by AspenTech

System modeled



10 species
50000 variables
Steady-state

Thermodynamic calls

- **gPROMS model calling A+ CO Property Package**
  - **Properties requested from Aspen Plus**
    - Vapor Heat Capacity
    - Vapor Thermal Conductivity
    - Vapor Enthalpy
    - Liquid Activity Coefficient
    - Liquid Enthalpy
    - Liquid Volume
    - Liquid Thermal Conductivity
    - Surface Tension
    - Liquid Fugacity Coefficient
    - Liquid Viscosity

    (note: flash equations within the gPROMS model)

Calls to CO Property Package

```
UNIT
      Plant AS Column
SET
      WITHIN Plant DO
         PhysProps := "(PS)ATCOProperties.COPropertySystem.1<gPROMS121new>";
……….
FOR y := 0 TO 1 DO
    FOR z := 0 TO 1 DO
        FOR i := 1 TO 4 DO
              Molarfrac_aux(i, y, z) = Molarfrac(i, y, z) ;
        END
        FOR i := 5 TO 11 DO
           Molarfrac_aux(i, y, z) = 0 ;
        END
        FOR i := 1 TO NoVapSpecies DO
          VapHeatCapacity(i, y, z) = PhysProps.VapourHeatCapacity(T(y, z), P, frac(i, )) ;
        END
          Lambda_vapour(y, z) = PhysProps.VapourThermalConductivity(T(y, z), P,
                                Molarfrac_aux(, y, z)) ;
    END
END
```

gO:CAPE-OPEN overview

- Introduce advanced gPROMS models within CAPE-OPEN compliant steady-state flowsheeting packages e.g.
  - ASPEN PLUS™
  - HYSYS™
- Use consistent physical properties throughout
- No programming required
  - retain advantages of gPROMS-based modelling

gPROMS model in Aspen Plus

- Creation of .gCO file from model file (copy and paste)
  - XML file containing
    - Ports information
    - Model
    - Behavior of UNIT operation
- Definition of Thermo server
  - PhysProps AS FOREIGN_OBJECT "gCOUnitThermo"

CAPE-OPEN UNIT objects

- A “CO unit object” may be
  - a single unit operation
  - a plant sub-section
  - a whole plant
- …connected to its environment via “ports” carrying material, energy or information
  - input ports
  - output ports
- …and characterised by “parameters”
  - input parameters
  - output parameters
- Unit object behaviour
  - given input port information and input parameter values
  - compute output port information and output parameter values

Definition of ports

```
<Ports>
    <Port Name="L_Feed">
        <Direction>Inlet</Direction>
        <Connectivity>Obligatory</Connectivity>
    </Port>
  <Port Name="V_Feed">
        <Direction>Inlet</Direction>
        <Connectivity>Obligatory</Connectivity>
    </Port>
  <Port Name="L_Prod">
        <Direction>Outlet</Direction>
        <Connectivity>Obligatory</Connectivity>
    </Port>
  <Port Name="V_Prod">
        <Direction>Outlet</Direction>
        <Connectivity>Obligatory</Connectivity>
    </Port>
</Ports>
```

Model imported from ModelBuilder

```
<gPROMSModel>
    <Activity>Simulation</Activity>
    <Password>$$WOmbat$</Password>
    <ProcessName>TEST_COLUMN</ProcessName>
    <gPROMSInputFile Name="Test_column_new.gPROMS">
      <Directory>input</Directory>
      <Body><![CDATA[
{
 gPROMS input file generated by gPROMS ModelBuilder 2.3.0
 Wed Jan 28 17:38:23 CET 2004
 AtofinaColumn -> file:/C:/Documents and
   Settings/PONS/Bureau/TOTAL/AtofinaColumn.gPJ
```

Demo

- Open an Aspen Plus data file
  - ➲ **Four material streams already defined**
- Choose gO:CAPE-OPEN unit operation
- Drop it on the palette
- Connect material streams to unit ports
- Define / change unit parameters
- Solve process model
- View results

Known problems

- gPROMS CO Unit was making a Pressure-Enthalpy flash on outlet streams:
  - Aspen Plus reported severe errors on these flashes
- gPROMS CO Unit now is making Pressure-Temperature flashes on outlet streams:
  - Aspen Plus now reports only mild warnings
- Other issues:
  - How automatically recognize chemical compounds?
  - Check/compute state of input feeds?
  - Incomplete usage of thermo properties provided by CO PP

Conclusion on gPROMS-Aspen Plus

- A gPROMS model may make use of a CO Property Package for thermodynamic and physical properties.
- No apparent performance degradation.
- The same gPROMS model may be transformed into a CO Unit Operation to be embedded in an Aspen Plus process model.
- It works!!!

Perspectives

- Fill the gap between detailed modelling and process simulation
- Relies on industry defined and supported interface standard (CAPE-OPEN)
- More tests / developments / improvements needed
- Chosen as solution for absorption modelling within ATOFINA

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