# Modeling Multicomponent Distillation with Open Source and CAPE-OPEN

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Gustavo León [a,b] / César Pernalete [b]

[a] Universidad de Los Andes (ULA)
[b] PDVSA Intevep


Gobierno Bolivariano de Venezuela | Ministerio del Poder Popular de Petróleo y Minería

- DWSIM, main features
- Methodology applied
- Cases of study
- Results
- Conclusions

# DWSIM, general overview

DWSIM
THE OPEN SOURCE CHEMICAL PROCESS SIMULATOR

GPL v3 Free Software

GPL v3 Licensing

**...offers freedom for:**

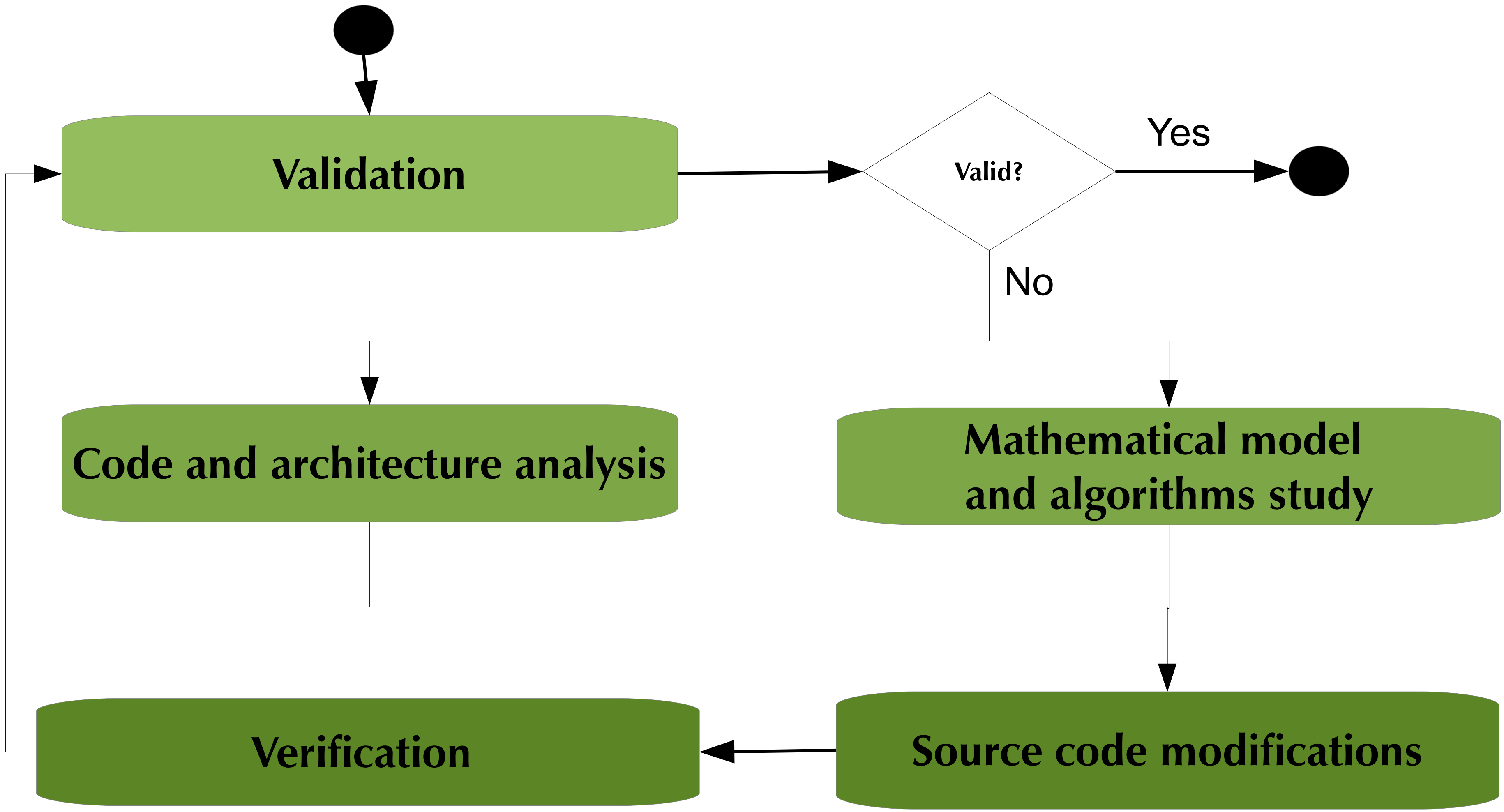
Using
Distribution
Source code access
Modification

Compliant with open standards CAPE-OPEN

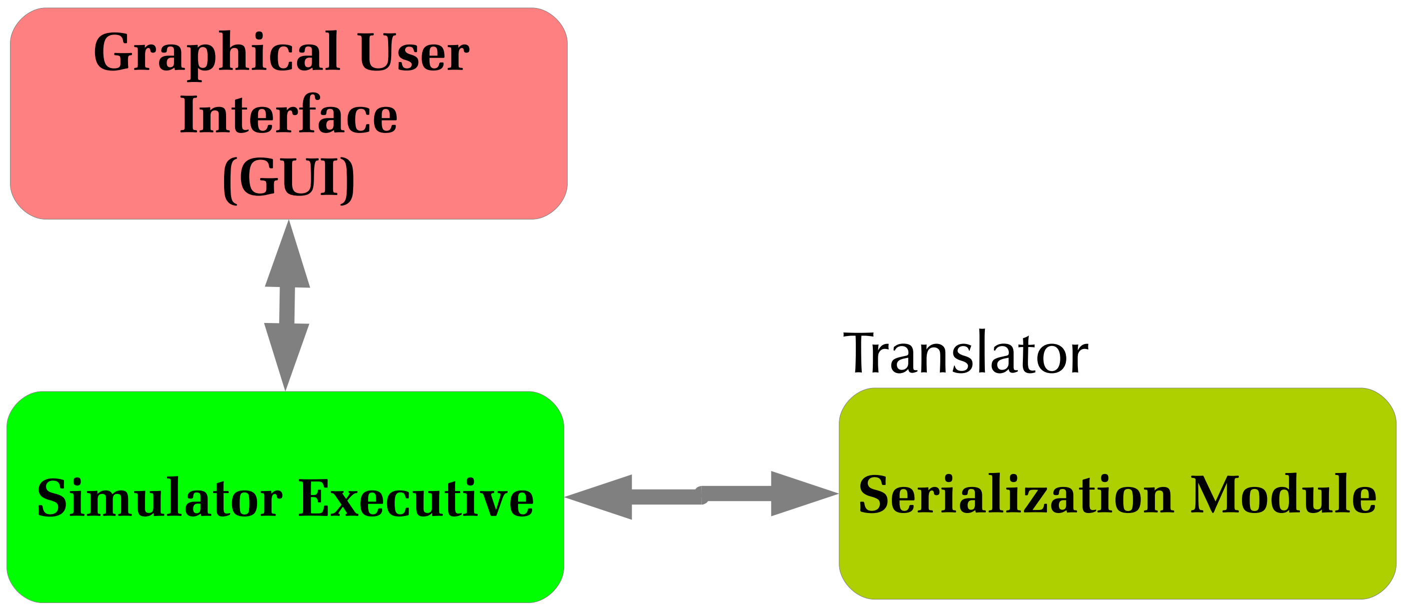
**...is able to communicate with:**

Commercial or non-commercial simulators
In house models
Another open source simulator

# Methodology applied



# General architecture



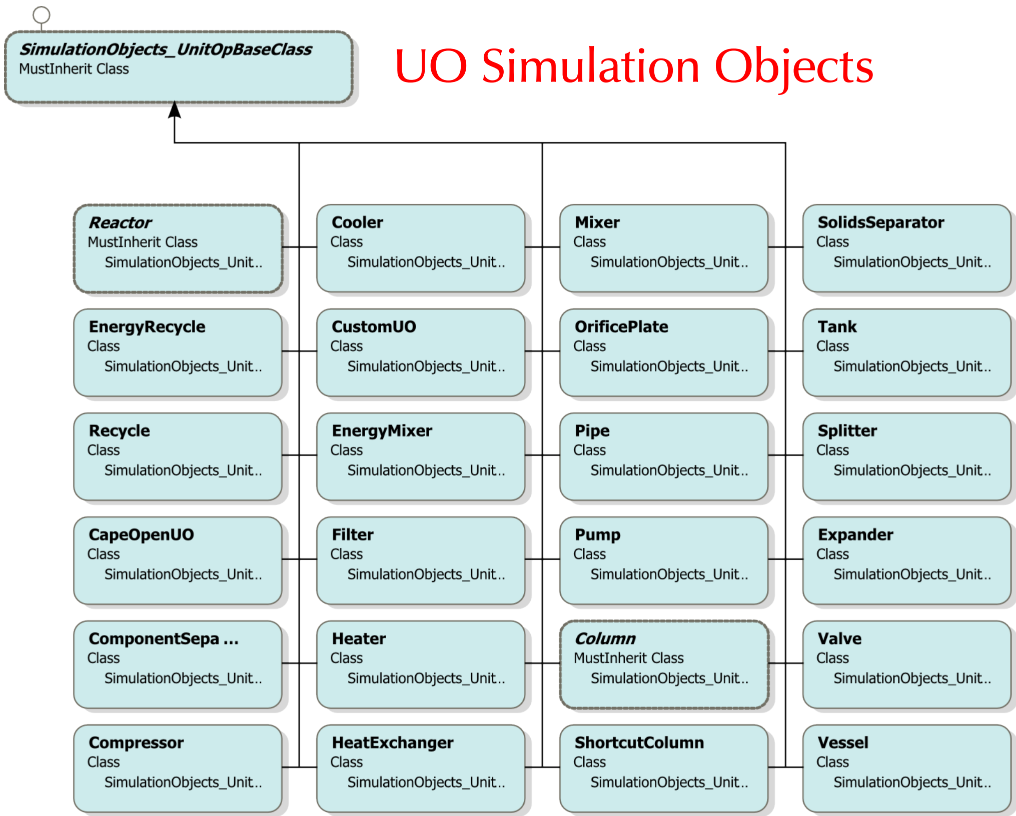

Main component

Thermodynamics
Unit Operations
Properties calculation

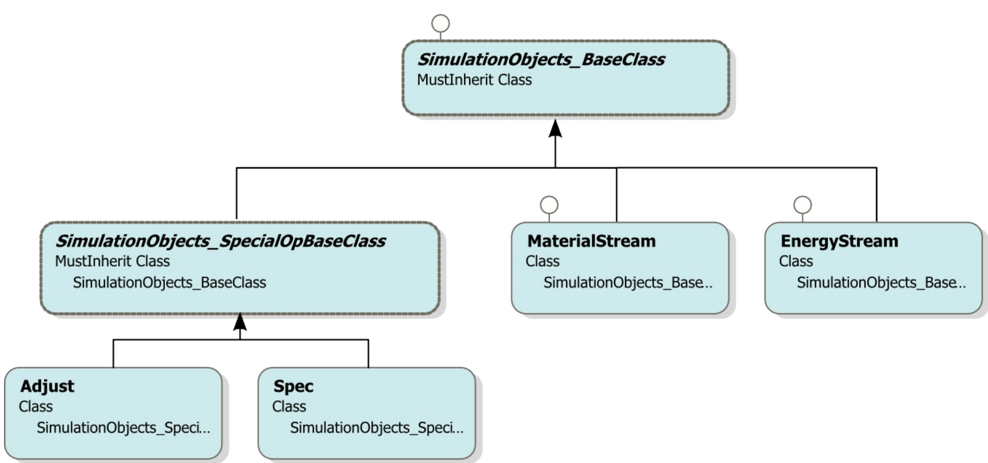
# Simulator Executive

## Object Oriented Architecture

UO Simulation Objects




Simulation Objects
Energy and material streams



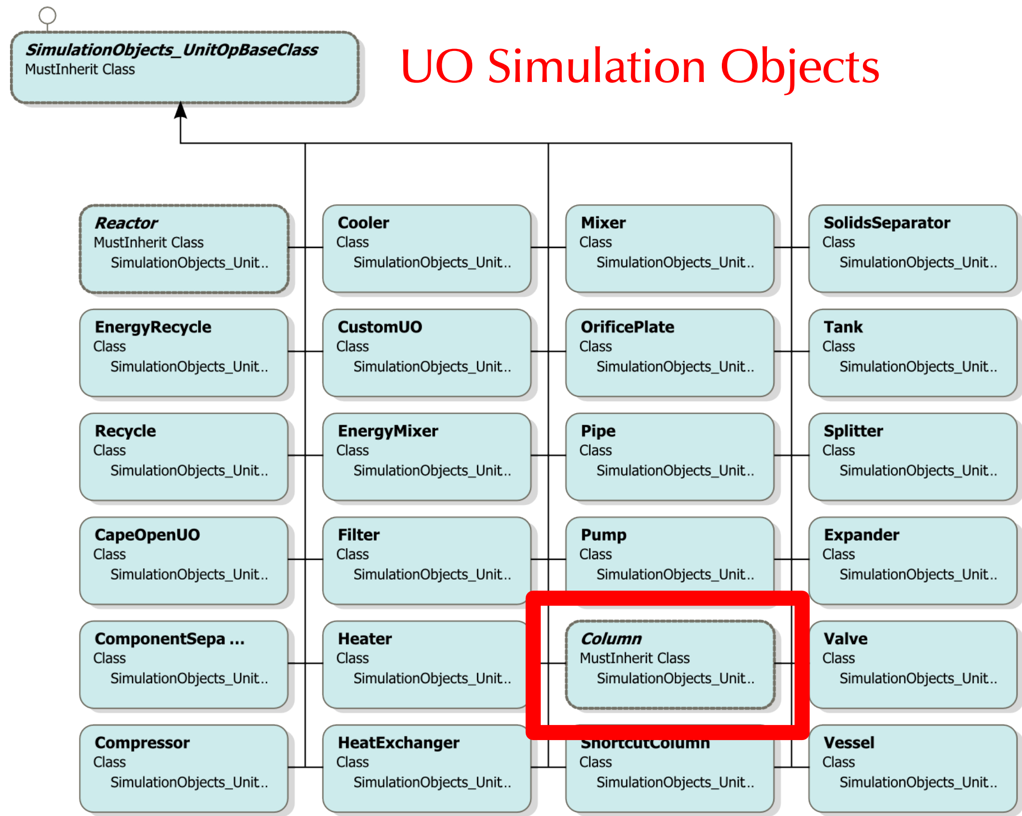


Thermodynamic property packages

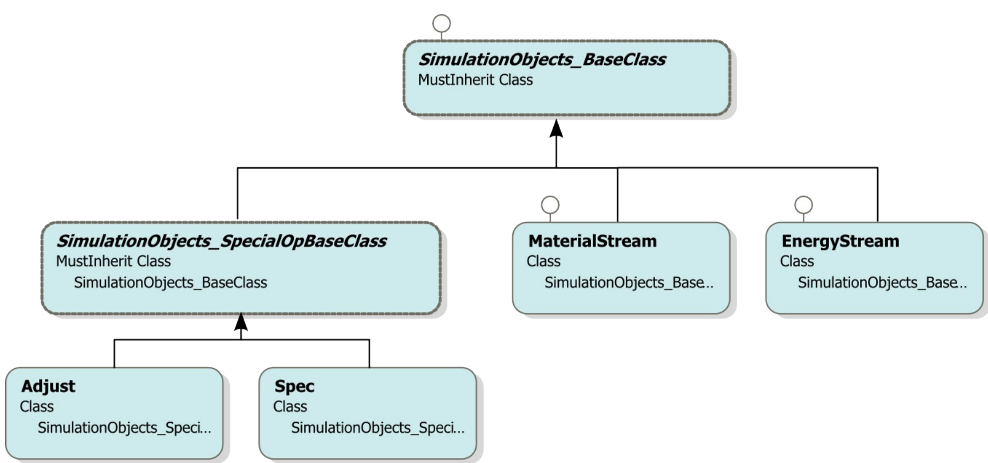
**Simulator Executive**

# Object Oriented Architecture

UO Simulation Objects




Simulation Objects
Energy and material streams

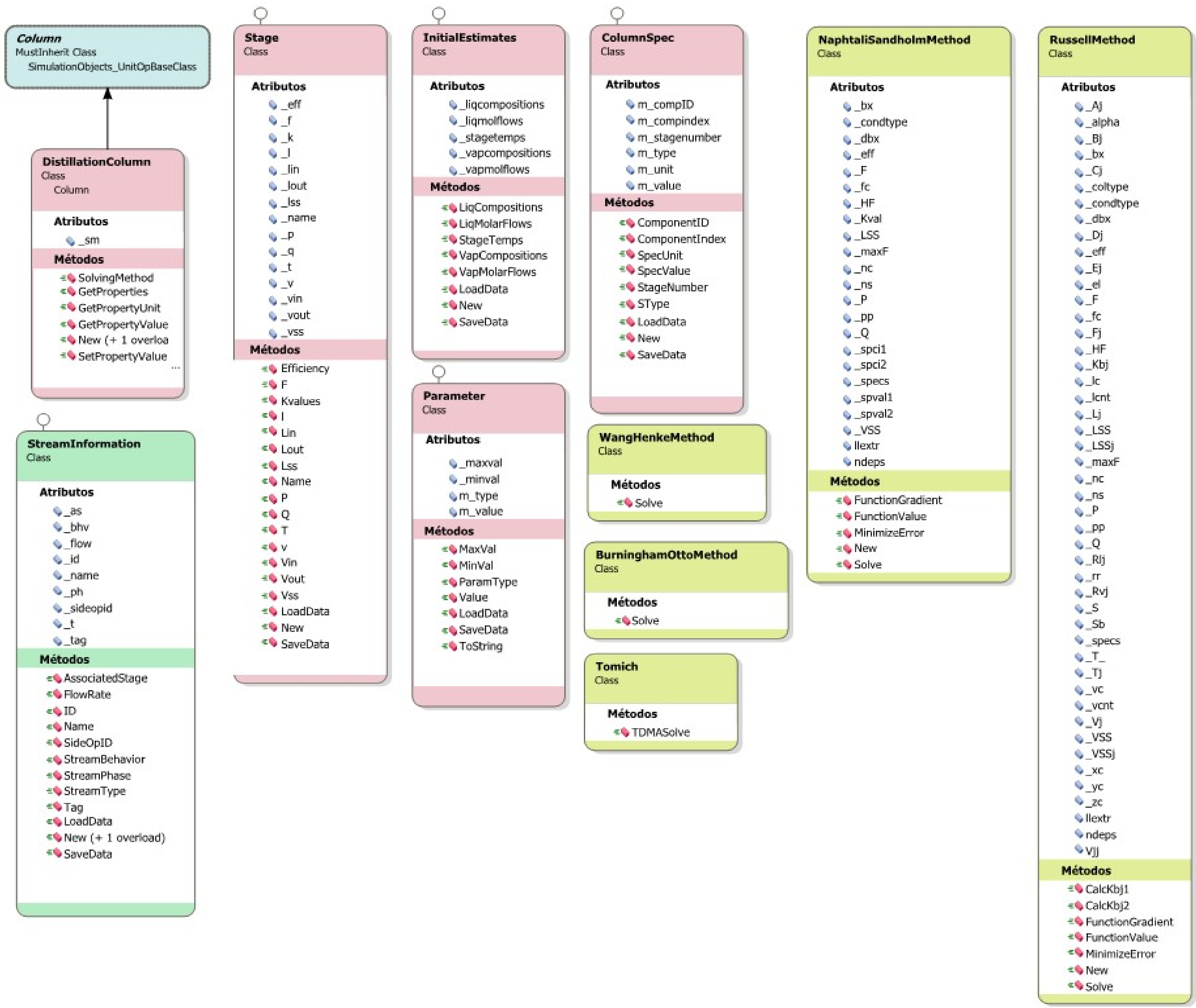




Thermodynamic property packages

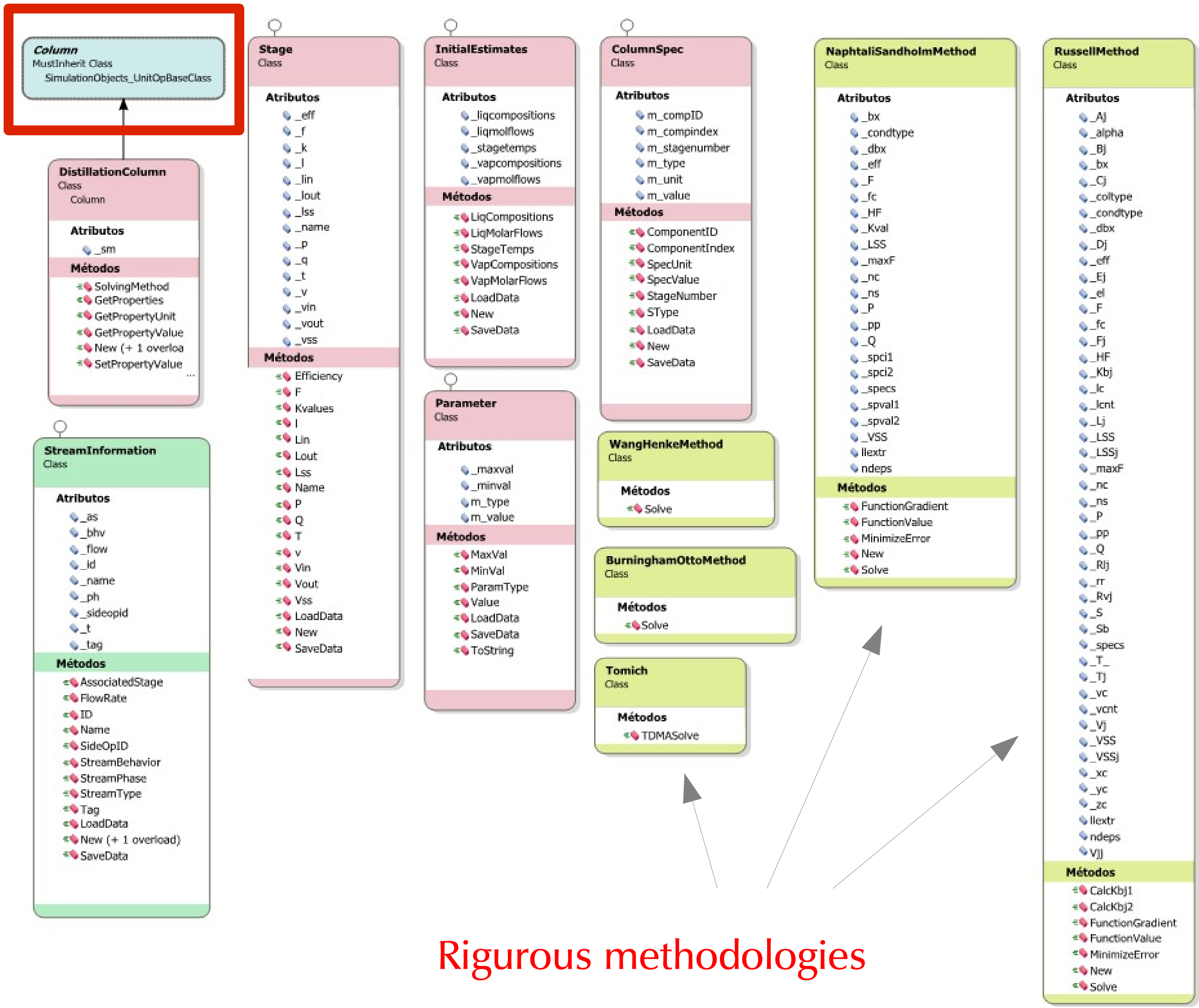
## Simulator Executive

Classes and methods were identified



# Simulator Executive

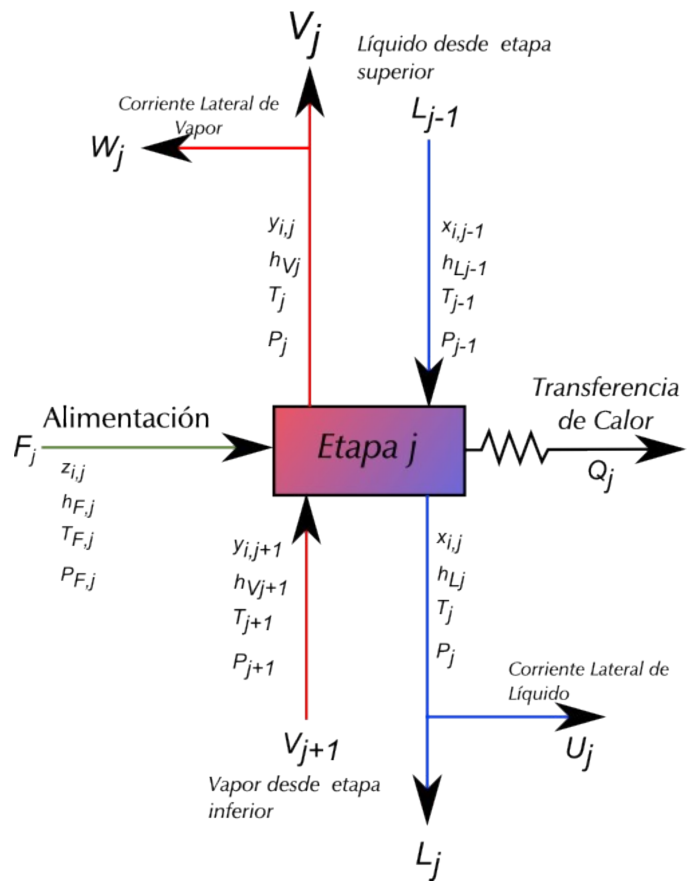
Classes and methods were identified

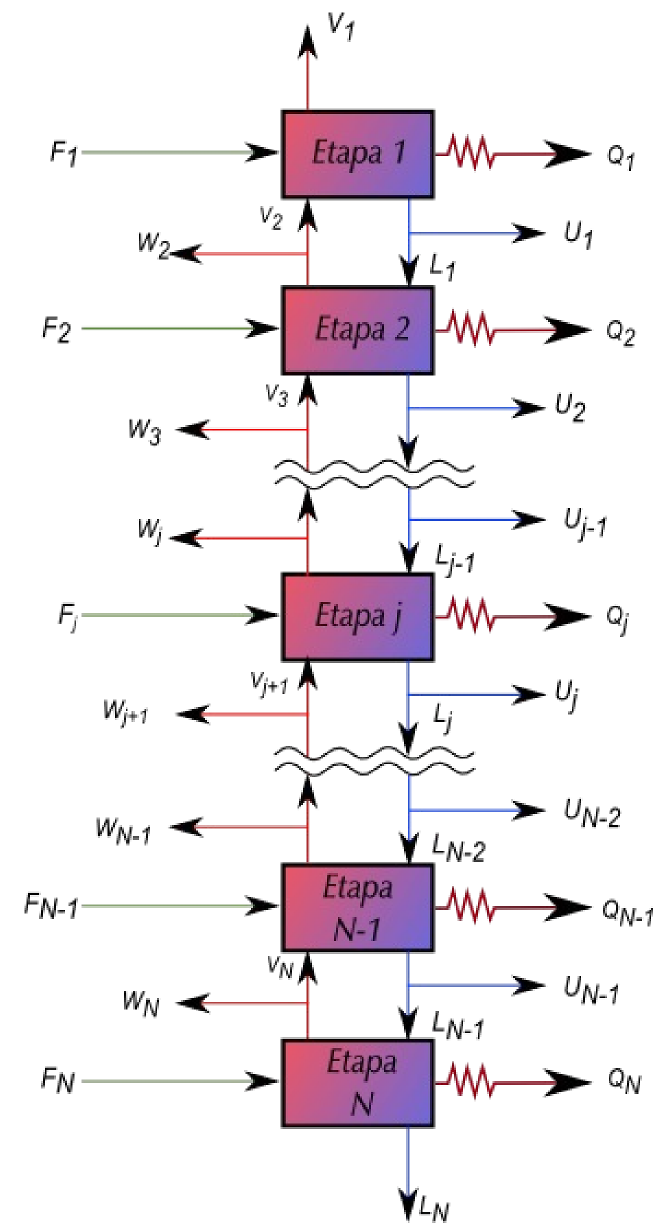


# The column model

## Equilibrium Stage Model

A column is the combination of different stages.



# The column model

**Model built using the MESH equations**

Non-linear relationships

Equations must be solved using numerical algorithms.

The Inside-Out method proposed by Russell (1983) was considered.

$$M_{i,j} = L_{j-1} x_{i,j-1} + V_{j+1} y_{i,j+1}$$
$$+F_j z_{i,j} - (L_j + U_j)\, x_{i,j} - (V_j - W_j)\, y_{i,j} = 0$$

$$E_{i,j} = y_{i,j} - K_{i,j} x_{i,j} = 0$$

$$(S_y)_j = \sum_{i=1}^{c} y_{i,j} - 1{,}0 = 0$$
$$(S_x)_j = \sum_{i=1}^{c} x_{i,j} - 1{,}0 = 0$$

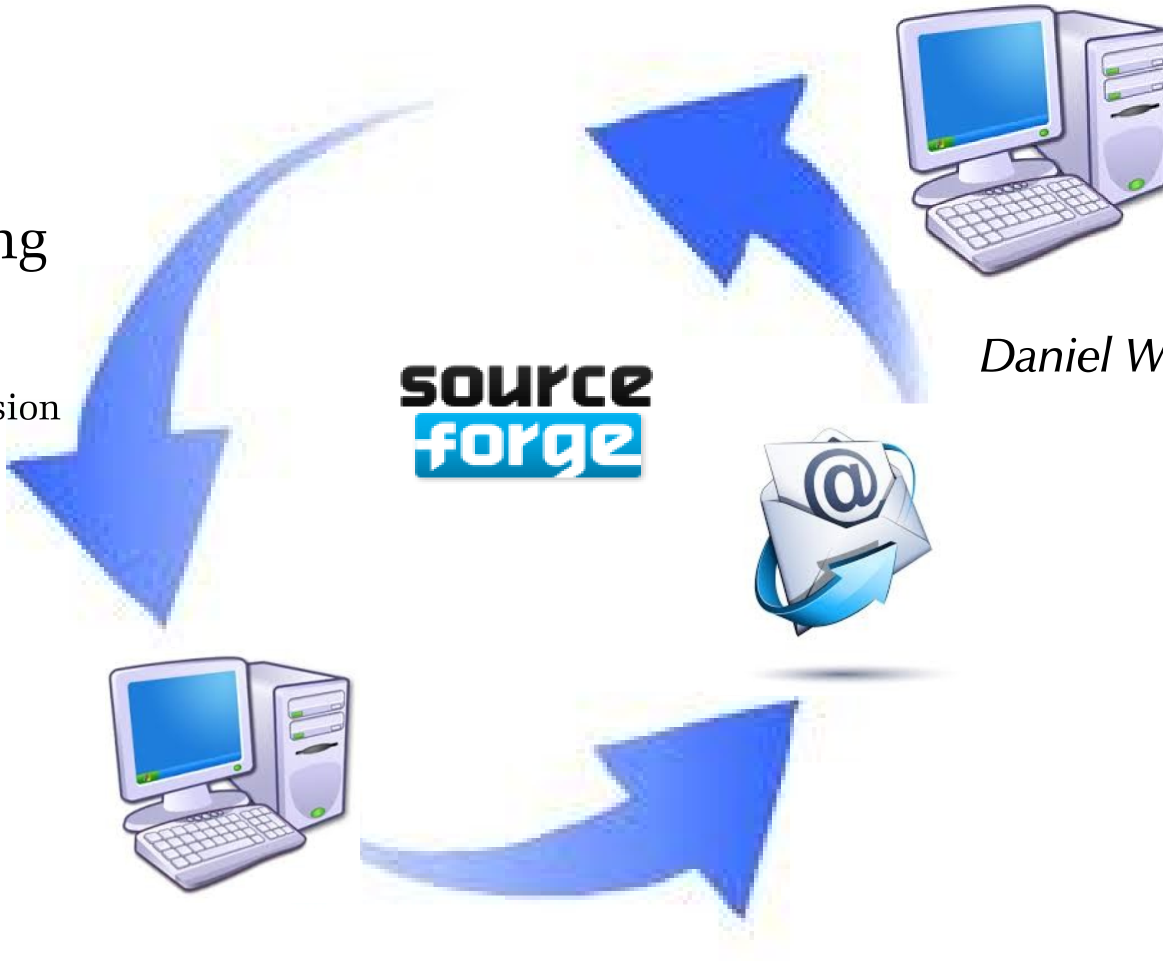
$$H_j = L_{j-1} h_{L_{j-1}} + V_{j+1} h_{V_{j+1}} + F_j h_{F_j}$$
$$-(L_j + U_j)\, h_{L_j} - (V_j + W_j)\, h_{V_j} - Q_j = 0$$

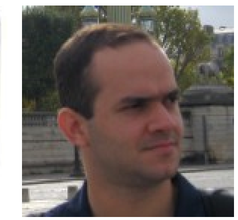
# Source code modifications

**Contact with the main developer of DWSIM**

Discussions in developing forums.

http://sourceforge.net/p/dwsim/discussion



*Daniel Wagner*

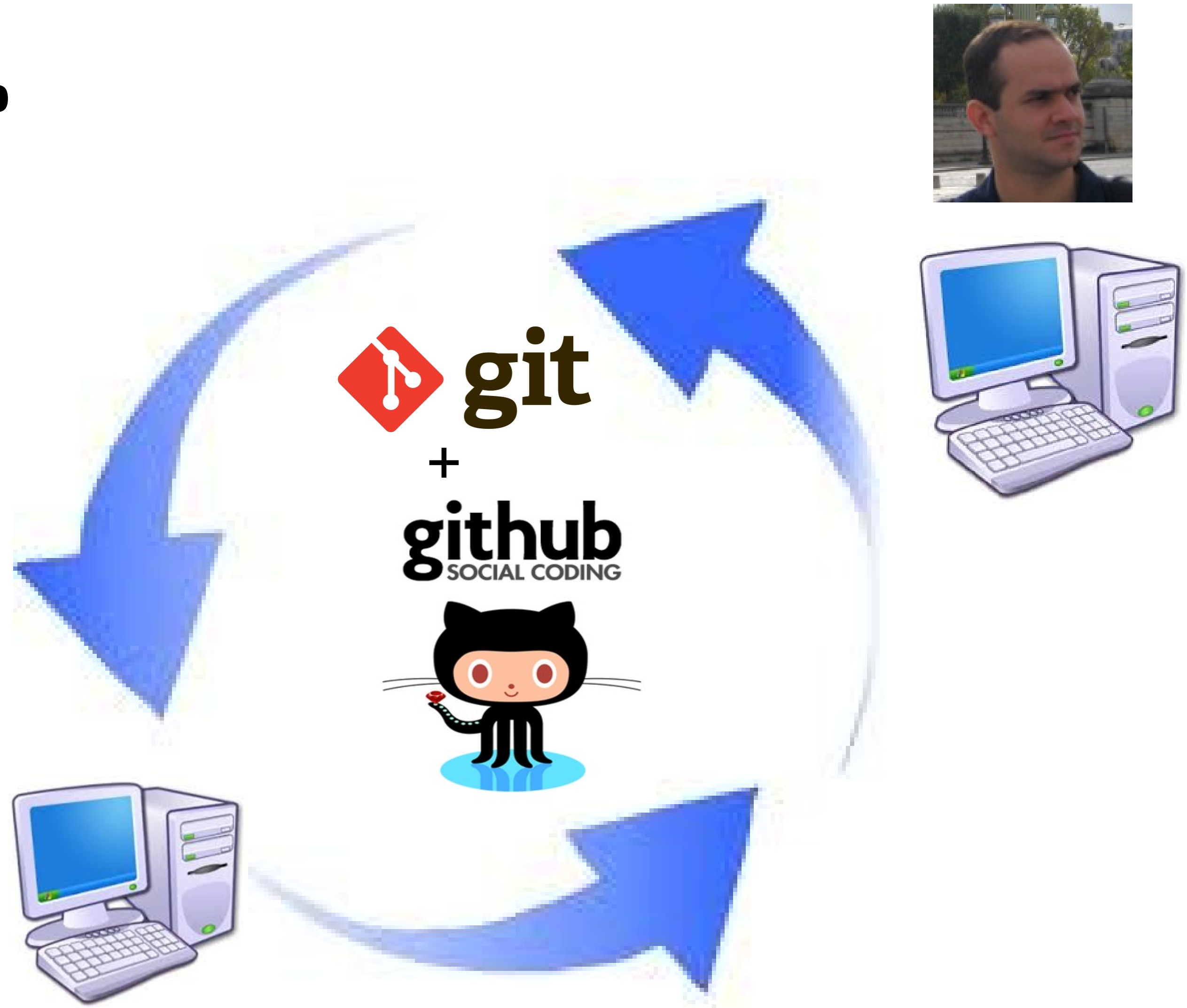
*César Pernalete*

*Gustavo León*

# Source code modifications

## Code Control using github

```diff
+               'Condenser Specs
                Select Case _specs("C").SType
                    Case ColumnSpec.SpecType.Component_Fraction
-                       If _specs("C").SpecUnit = "M" Then
-                           spfval1 = -_xc(0)(spci1) + spval1
-                       Else 'W
-                           spfval1 = -_pp.AUX_CONVERT_MOL_TO_MASS(_xc(0))(spci1)
+                       If _condtype = Column.condtype.Total_Condenser Then
+                           If _specs("C").SpecUnit = "M" Then
+                               spfval1 = _LSSj(0) * _xc(0)(spci1) - _LSSj(0) * s
+                           Else 'W
+                               spfval1 = _pp.AUX_CONVERT_MOL_TO_MASS(_xc(0))(spc
+                           End If
+                       Else
+                           If _specs("C").SpecUnit = "M" Then
+                               spfval1 = _Vj(0) * _yc(0)(spci1) - _Vj(0) * spval
+                           Else 'W
+                               spfval1 = -_pp.AUX_CONVERT_MOL_TO_MASS(_yc(0))(sp
+                           End If
                        End If
                    Case ColumnSpec.SpecType.Component_Mass_Flow_Rate
-                       spfval1 = _LSSj(0) * _xc(0)(spci1) - spval1 / _pp.RET_VM
+                       If _condtype = Column.condtype.Total_Condenser Then
+                           spfval1 = _LSSj(0) * _xc(0)(spci1) - spval1 / _pp.RE
+                       Else
+                           spfval1 = _Vj(0) * _yc(0)(spci1) - spval1 / _pp.RET_
+                       End If
                    Case ColumnSpec.SpecType.Component_Molar_Flow_Rate
-                       spfval1 = _LSSj(0) * _xc(0)(spci1) - spval1 / _maxF
+                       If _condtype = Column.condtype.Total_Condenser Then
+                           spfval1 = _LSSj(0) * _xc(0)(spci1) - spval1 / _maxF
+                       Else
```




# Cases of study

**Verification**

## Open literature case

Light hydrocarbons columns

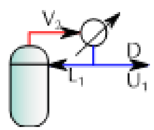
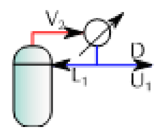
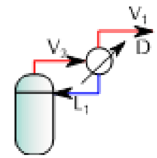
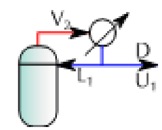
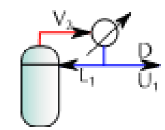
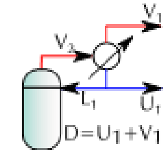
**Validation**

## Real operational case

Aromatic separation column
FCC Depropanizer column

# Cases of study

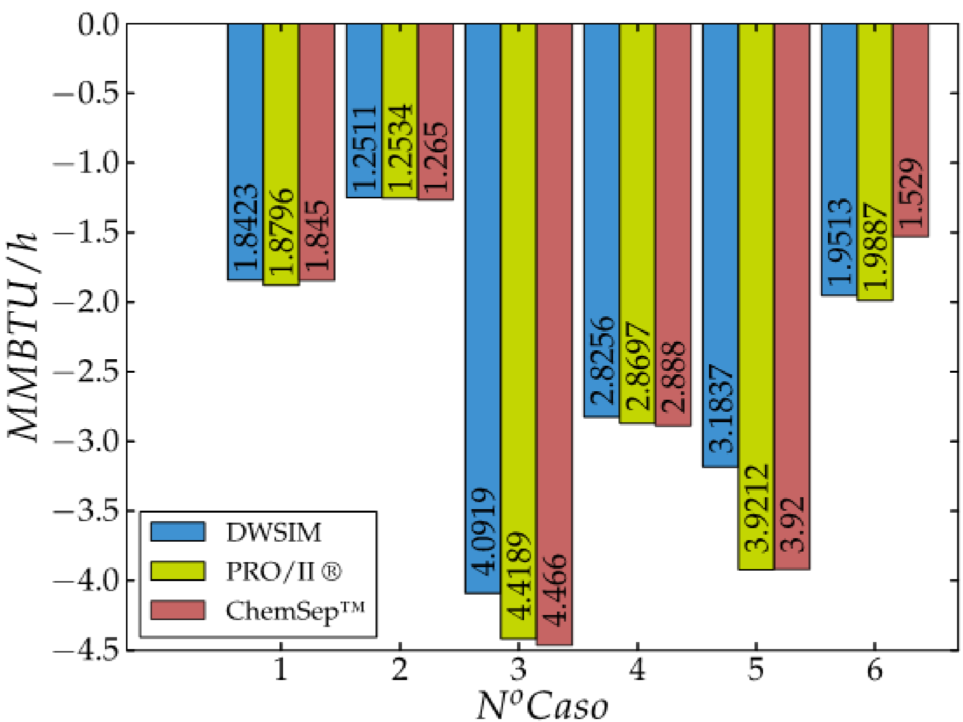
## Verification

| | Caso 1 | Caso 2 | Caso 3 | Caso 4 | Caso 5 | Caso 6 |
|---|---|---|---|---|---|---|
| *Presión de Columna (psi)* | 16,17 | 100,00 | 400 | 20 | 290,08 | 239,31 |
| *Número de Etapas de Equilibrio* | 10 | 5 | 13 | 30 | 31 | 16 |
| $\Delta P$ *Caída de Presión (psi)* | 0,00 | 0,00 | 0,00 | 5 | 0,00 | 0,00 |
| *Tipo de Condensador* | Total  | Total  | Full-Reflux  | Total  | Total  | Parcial  |

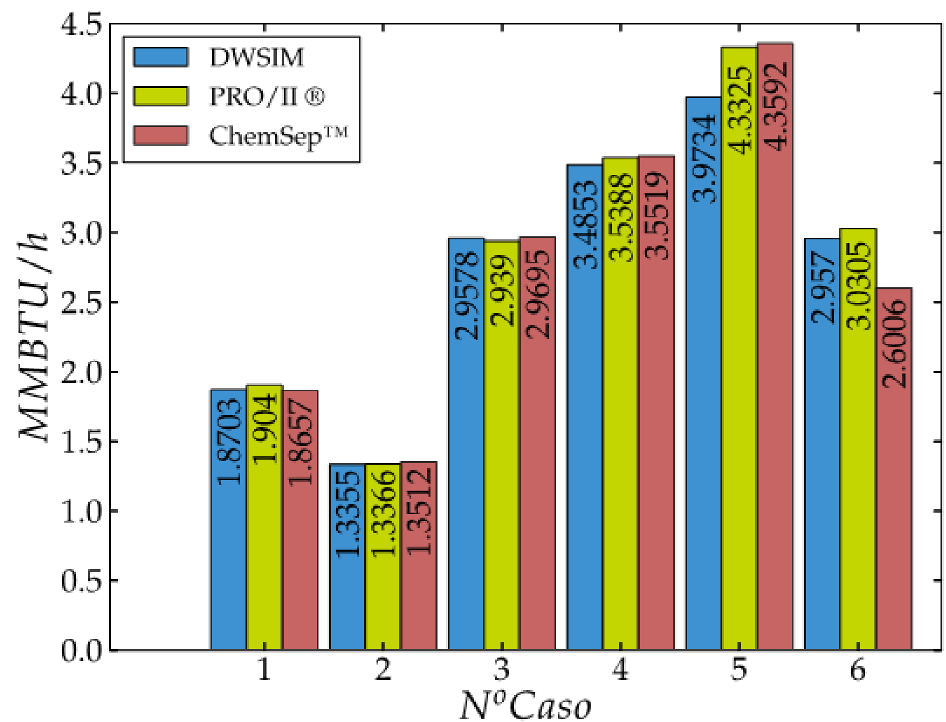
From Methane to Octane + Benzene + Toluene

# Cases of study

## Verification



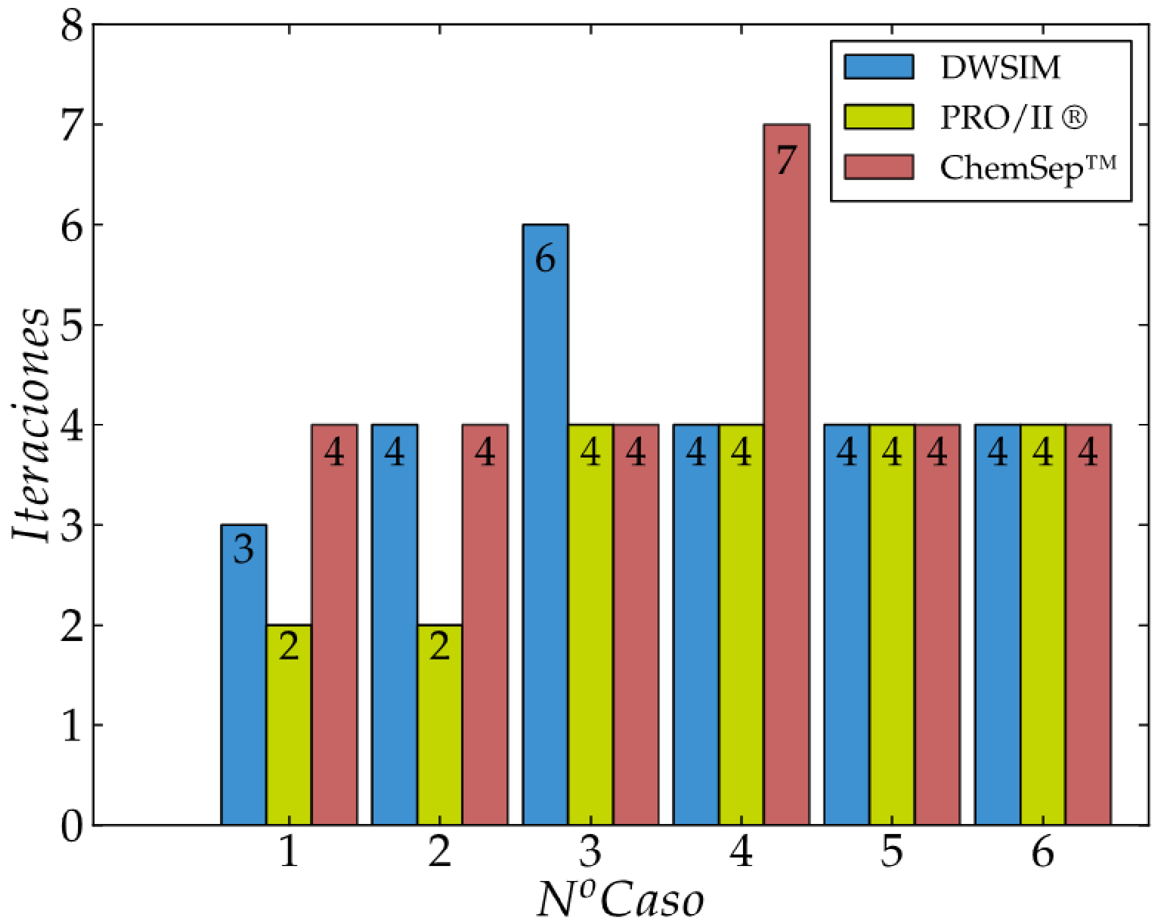

(a) Flujos de Calor de condensador




(b) Flujos de Calor de Rehervidor

# Cases of study

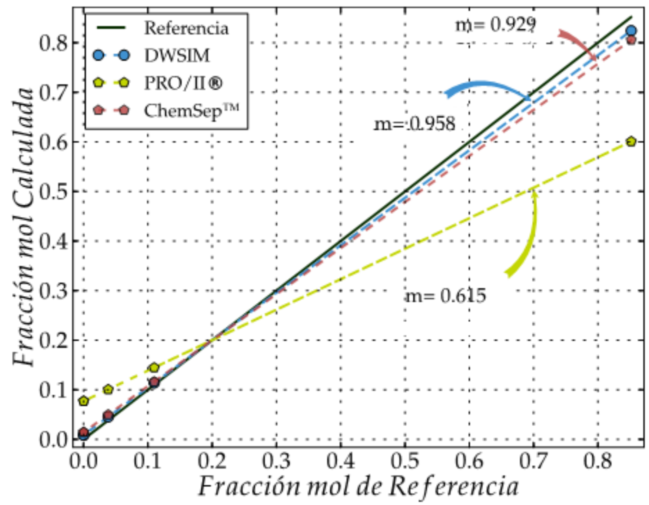
## Verification



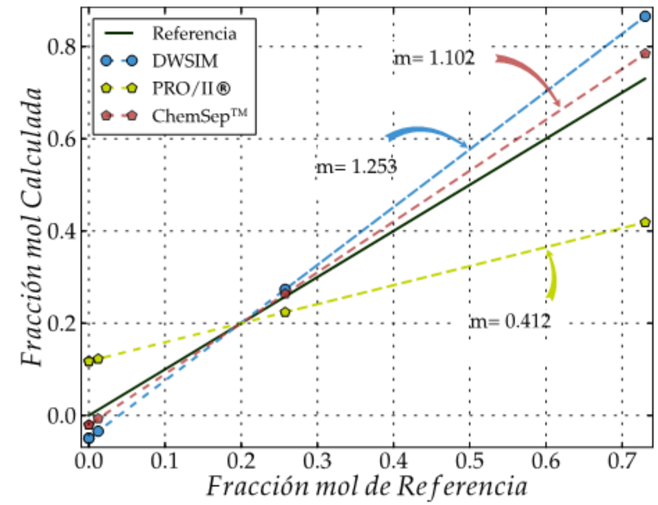
# Cases of study

## Verification

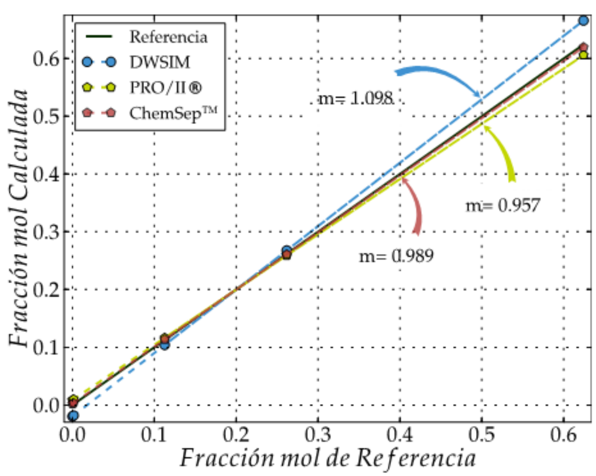
- **Case N°6**



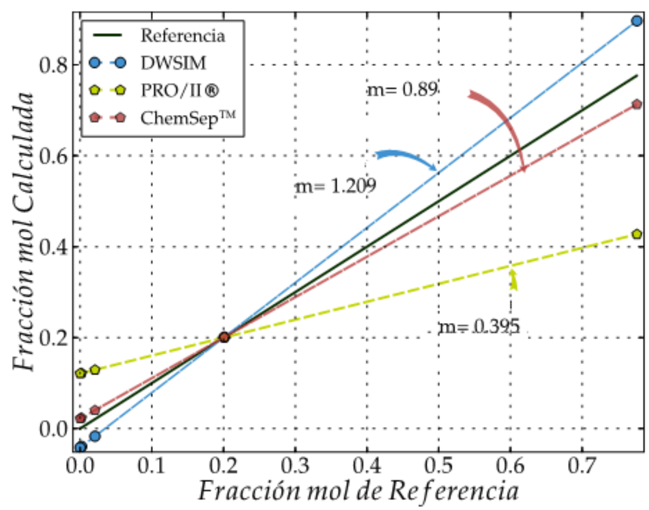

(a) Producto vapor de tope



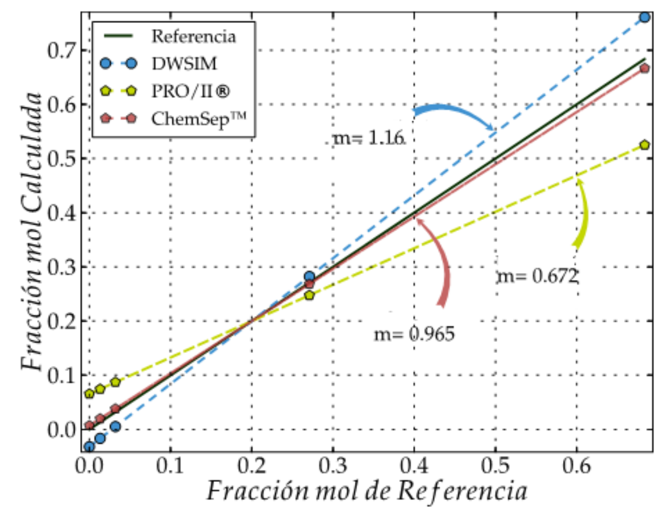

(b) Producto líquido de tope




(e) Producto líquido de fondo




(c) Retiro líquido lateral

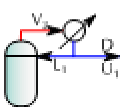
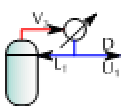



(d) Retiro vapor lateral

# Cases of study

## Validation

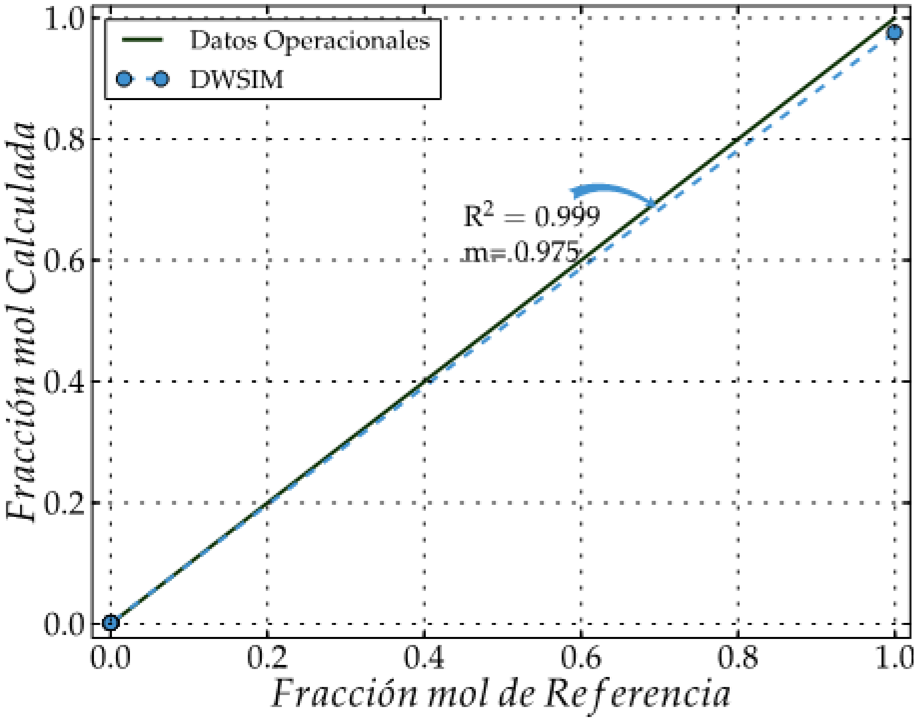
### Aromatics separator

| | Escenario 1 | Escenario 2 |
|---|---|---|
| $\triangle P$ ***Columna (psi)*** | 7 | 6 |
| ***Número de Etapas de Equilibrio*** | 40 | 40 |
| ***Tipo de Condensador*** | Total  | Total  |
| ***Presión de Condensador (psi)*** | 16,7 | 19,7 |
| ***Producto de Fondo*** (lb/h) | 36725,00 | 31970,00 |
| ***Relación de Reflujo*** | 4,4 | 4,55 |
| ***Flujo Total*** (lb/h) | 40035,81 | 44826,22 |
| ***Temperatura (°F)*** | 179,3 | 243,0 |
| *Etapa* | 17 | 17 |

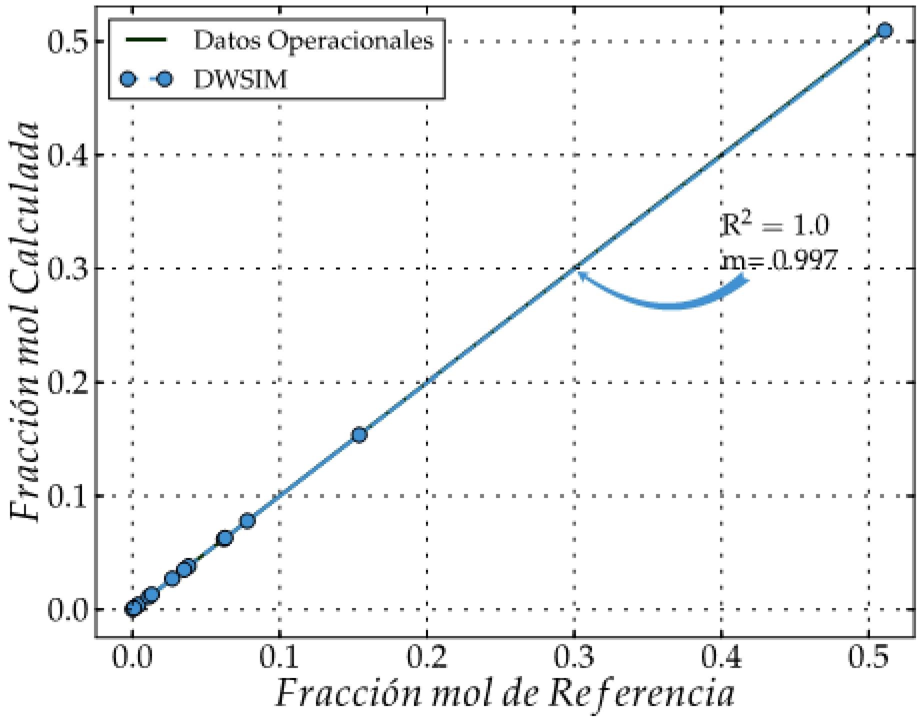
# Cases of study

## Validation

### Aromatics separator. Scenario #1




(a) Producto de Tope

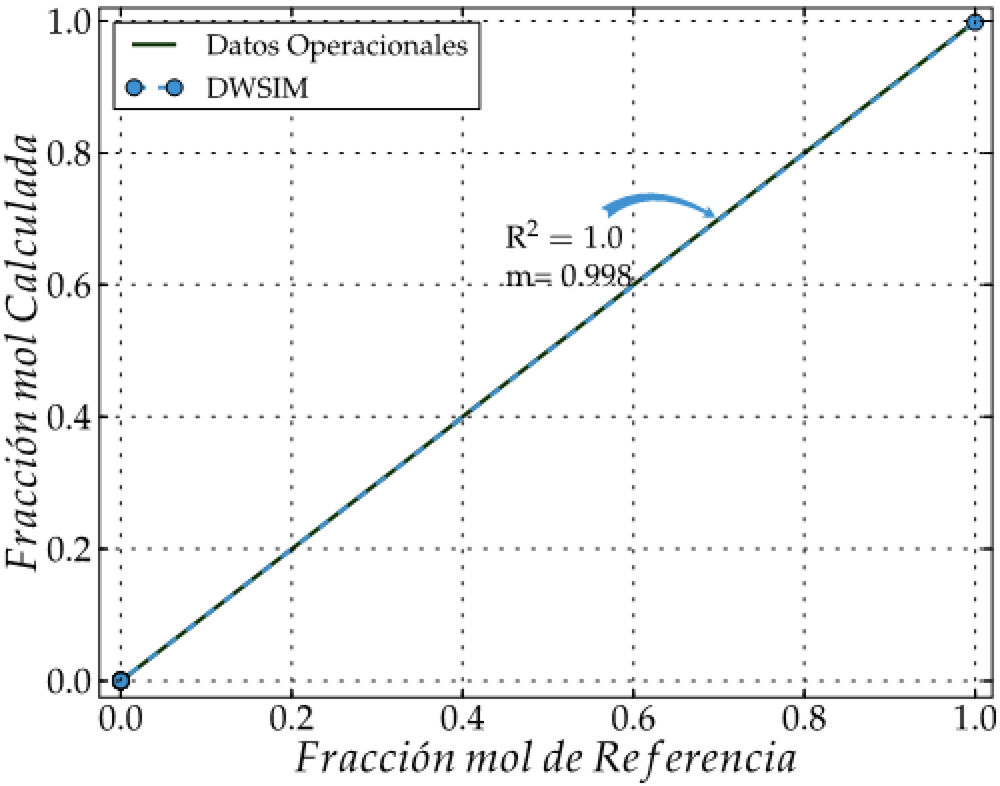



(b) Producto de Fondo

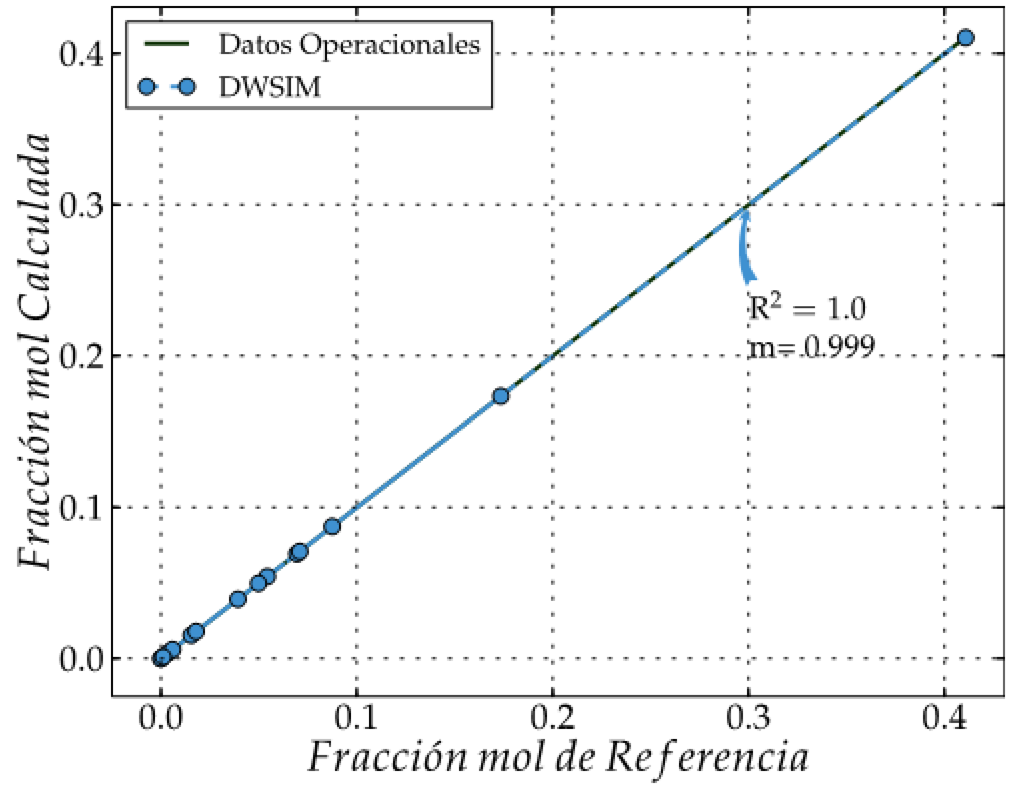
# Cases of study

## Validation

Aromatics separator. Scenario #2




(a) Producto de Tope

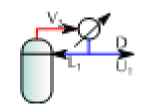



(b) Producto de Fondo

# Cases of study

## Validation

### FCC Depropanizer

| | |
|---|---|
| *$\Delta P$ Columna (kPa)* | 34,47 |
| *Número de Etapas de Equilibrio* | 30 |
| *Tipo de Condensador* | Total  |
| *Presión de Condensador (kPa)* | 1999,48 |
| *Producto de Fondo* $(kg/s)$ | 10,576 |
| *% Recuperación Propano* | 98,0 |
| *Temperatura (°C)* | 83 |
| *Presión (kPa)* | 2068 |
| *Etapa* | 14 |
| *Paquete Termodinámico* | CAPE-OPEN Peng-Robinson |

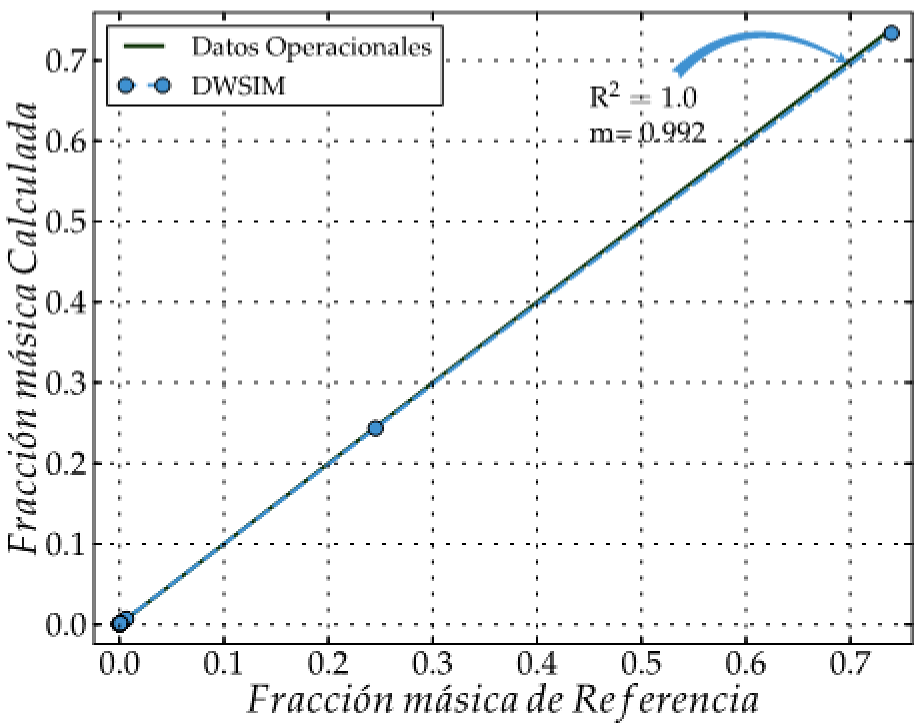
# Cases of study

## Validation

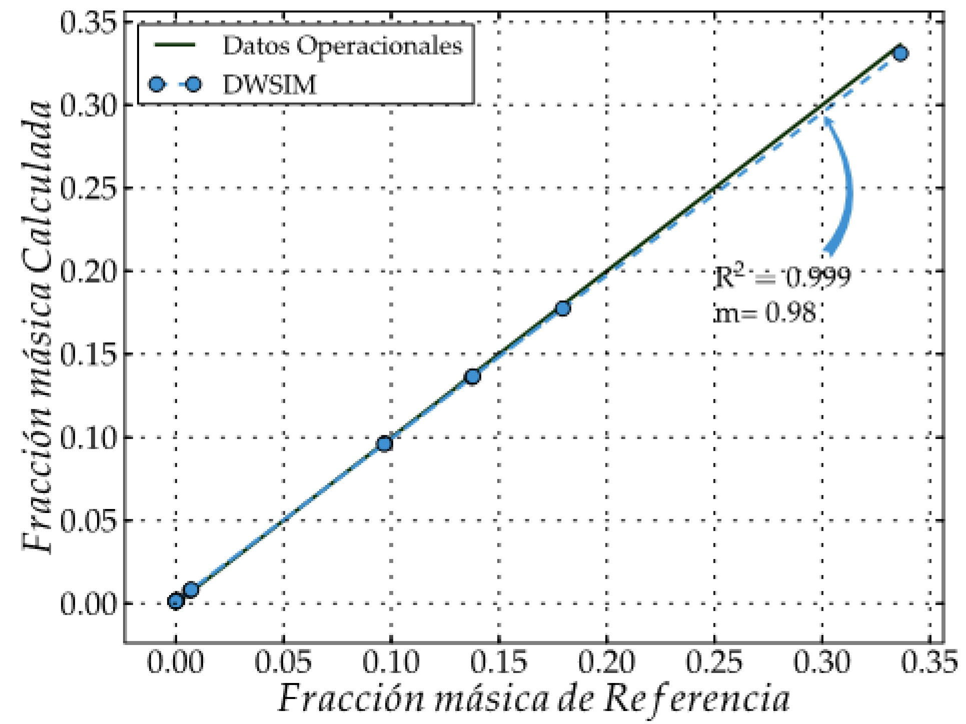
### Depropanizer

CAPE-OPEN

TEA




(a) Producto de Tope




(b) Producto de Fondo

# Conclusions

- All the elements that integrates DWSIM were identified.
- DWSIM was adapted sucessfully to simulate distillation columns in a PDVSA Refinery.
- Predictions were in good agreement with operational data.
- CAPE-OPEN allowed using an external thermodynamic when problems occurred in the native ELV calculations.
- DWSIM modifications were carried out colaborating through the open source community social networks.