



# Integrating a proprietary simulation tool into a commercial process simulator

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#### **EPC Work Flow**

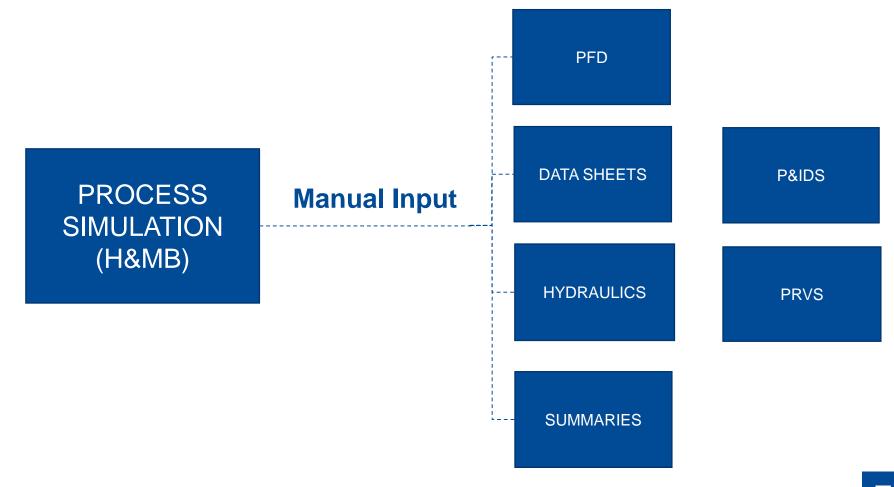






#### **Motivation**

#### **Basic Engineering Work Flow**







## Disadvantages of manual data transfer in current workflow

- Breaks the digitalization process/flow
- Engineering workflow interrupted
- Time and resource consuming
- Prone to errors and inconsistencies
  - During creation of heat and material balance
  - When processing change requests
- Complicates collaboration as a global team, if e.g.
  - Heat and material balance
  - Equipment data sheets are generated in different office locations

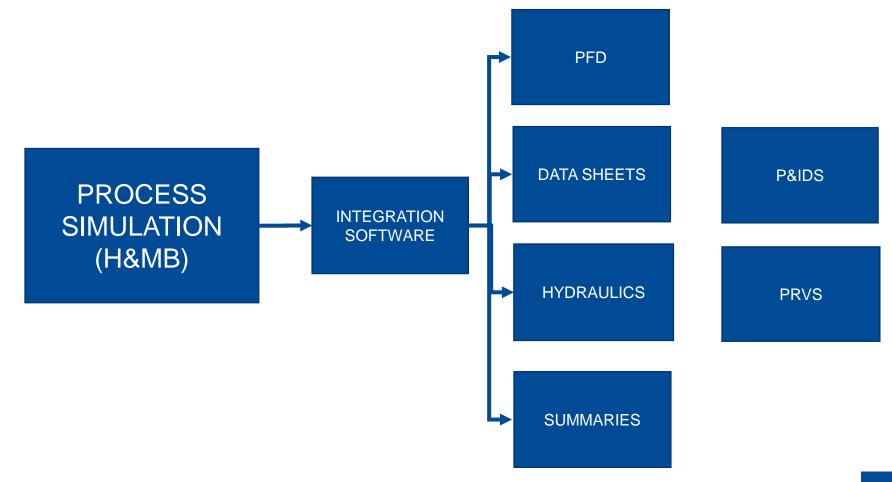






#### **Motivation**

#### **Basic Engineering Work Flow**

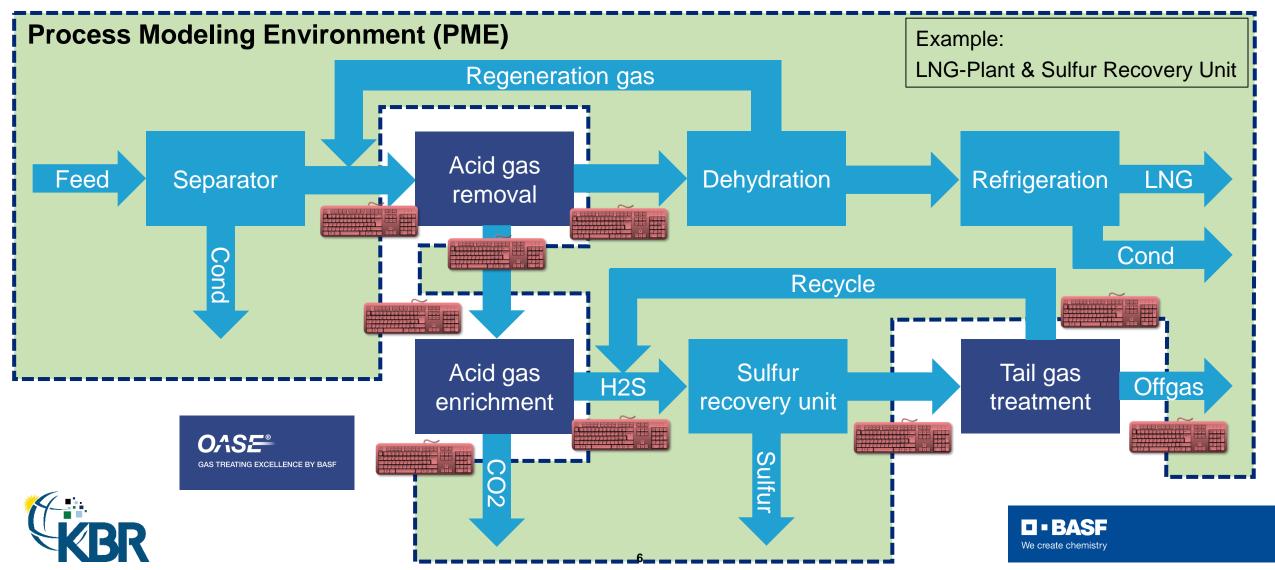




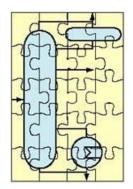


## Interaction with in-house or proprietary simulation tools in process

**simulation**  $\rightarrow$  Manual transfer of input and output data required



## **CAPE-OPEN**



#### The CAPE-OPEN Standard

- ... defines rules and interfaces that allow CAPE (Computer-Aided Process Engineering) applications to interoperate
  - Examples: Interfaces for thermodynamic models and for unit operations



- CO-LaN (<u>http://www.colan.org/</u>)
  - ... is a not-for-profit member society established in France in 2001
  - manages the CAPE-OPEN standard
  - In facilitates the implementation of CAPE-OPEN interfaces through software tools and services

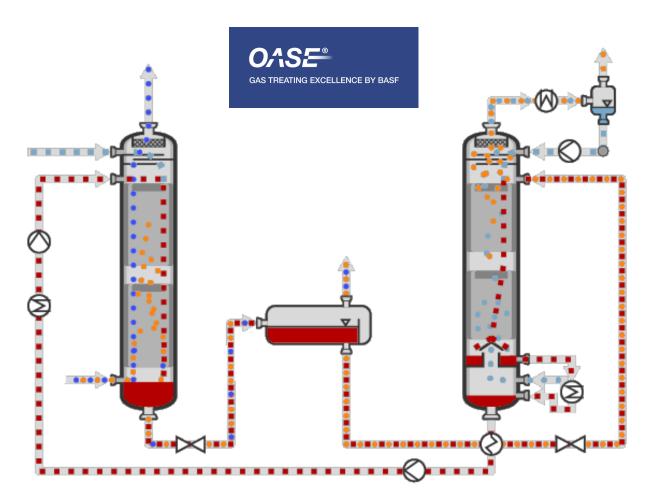


## **CAPE-OPEN** interfaces – What are we talking about?

| Process Modeling Environment<br>(PME)  | CAPE-OPEN interface                     | Process Modeling Component<br>(PMC)   |  |
|--|---|---|--|
| <ul><li>Software environment that supports</li><li>construction of a process model</li><li>process simulation or optimization</li></ul>  | Communication between CAPE applications | Software component, which is<br>intended to carry out a well-defined<br>function with limited scope |  |
| <ul> <li>Flow sheet simulator, e.g.</li> <li>Aspen Plus<sup>®</sup></li> <li>Aspen HYSYS<sup>®</sup></li> <li>COFE</li> <li>ProMax<sup>®</sup></li> <li>Pro/II</li> <li>UniSim<sup>®</sup> Design</li> <li></li> </ul> | Material Streams                        | <ul><li>Examples:</li><li>Computation of physical properties</li></ul>                              |  |
|  | Energy Streams                          | <ul> <li>Simulation of a particular unit<br/>operation</li> </ul>                                   |  |
|  | Parameters                              | <ul> <li>Numerical solution of certain<br/>types of mathematical problems</li> </ul>                |  |
| KBR  | Others<br>8                             | <b>D = BASF</b><br>We create chemistry  |  |

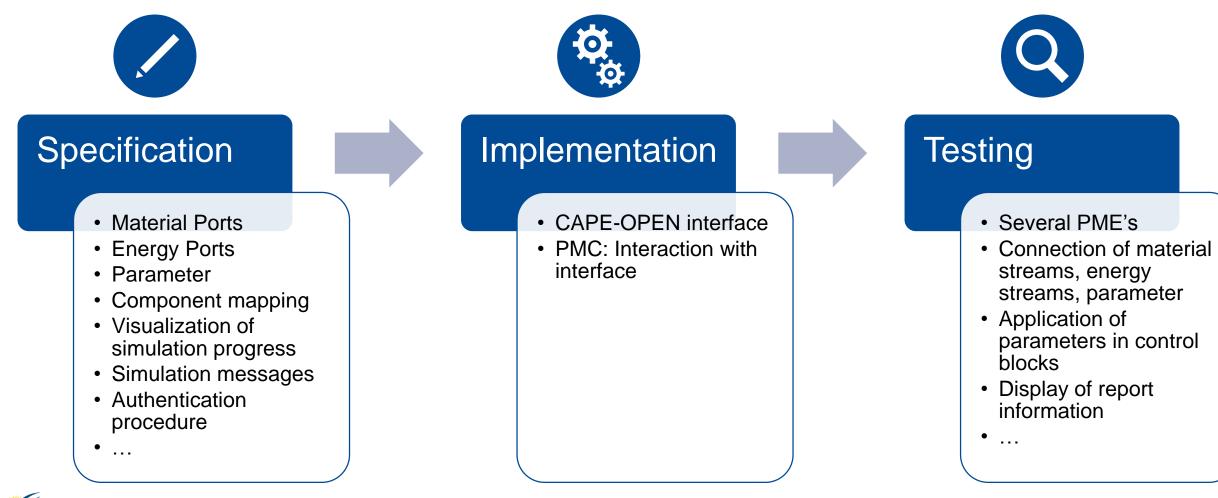
## **Example for PMC**

- BASF's OASE<sup>®</sup> gas treatment technology for removal of acid gases
- Acid gas removal unit (AGRU) is part of large production plants, e.g.
  - LNG plants / natural gas processing plants
  - Ammonia plants / synthesis gas plants
- Proprietary simulation tool OASE connect:
  - Allows rigorous calculation of BASF's OASE<sup>®</sup> gas treatment technology
  - Is provided as server client application



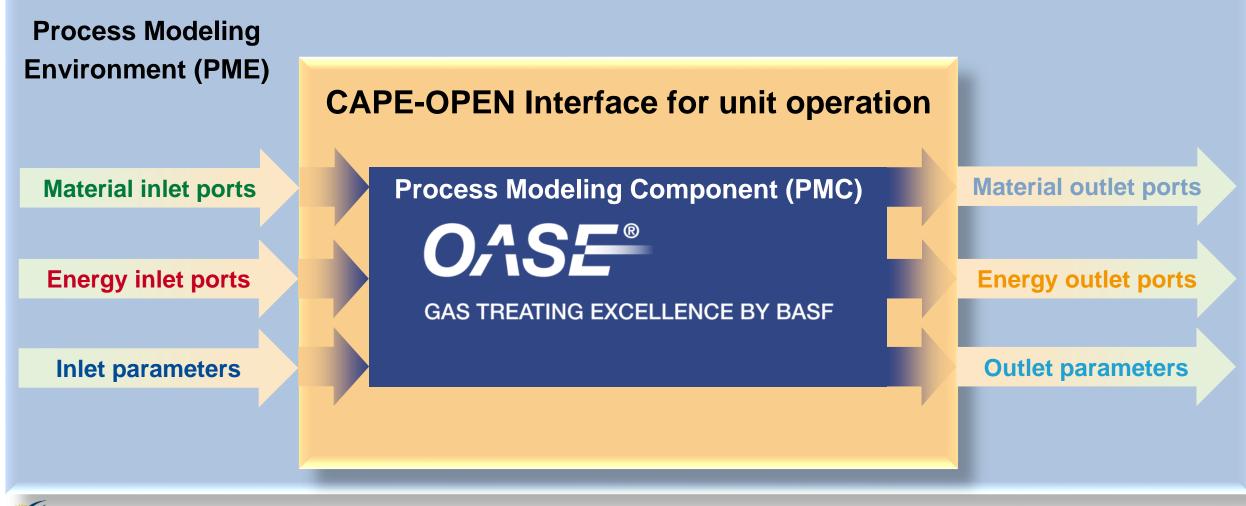


#### **Realization of CAPE-OPEN interface in OASE connect**





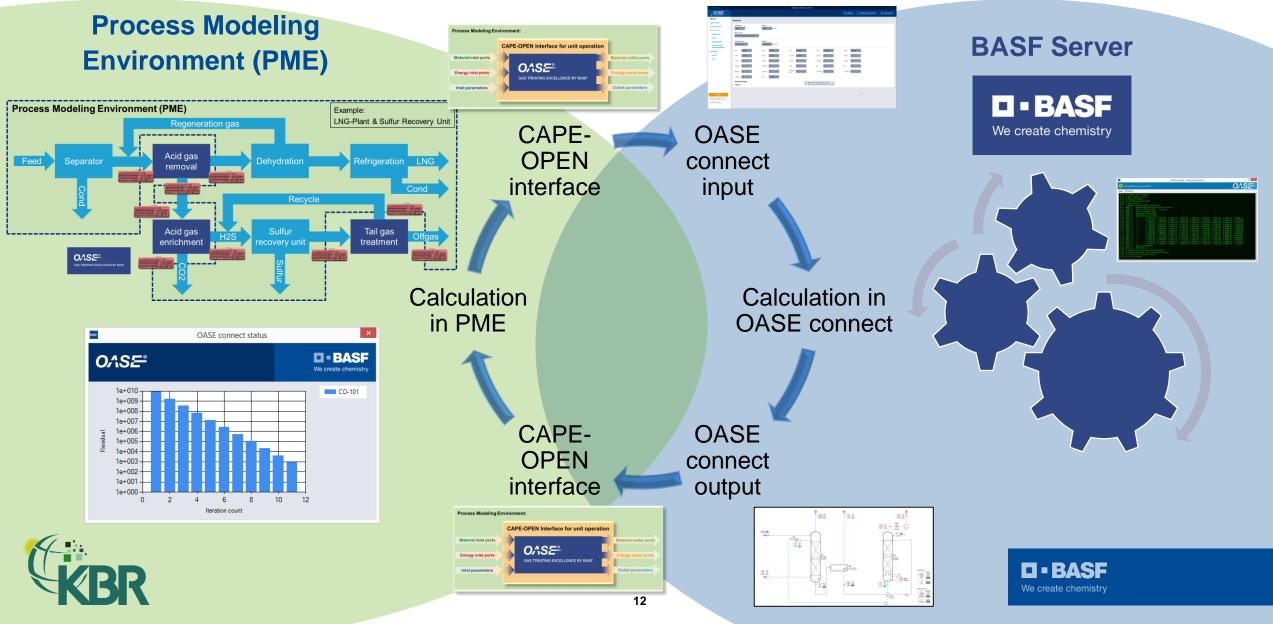
#### **CAPE-OPEN** interface allows communication between PME and PMC

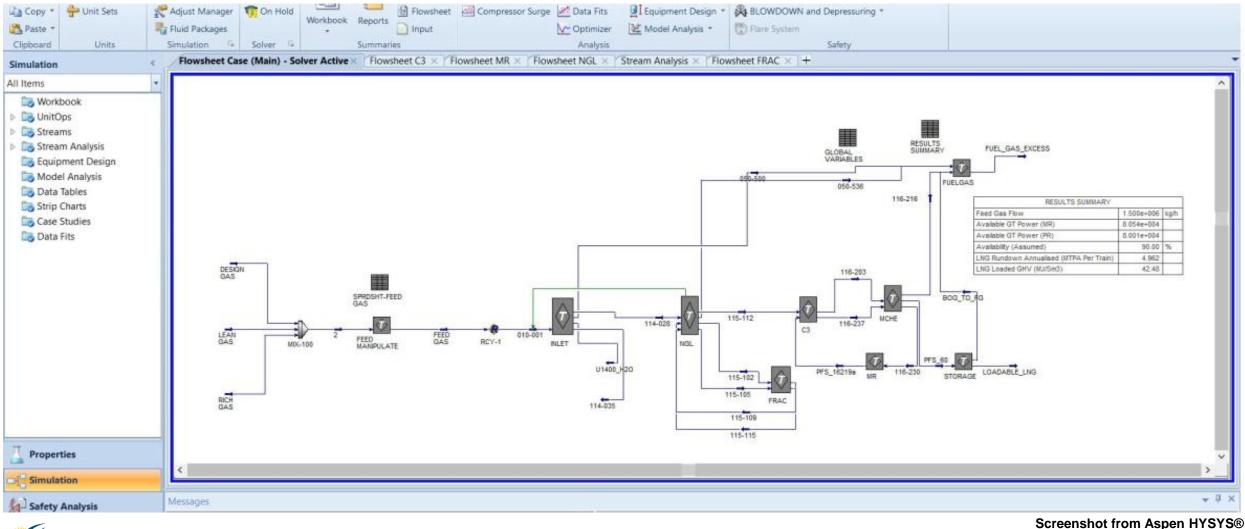






#### Interaction between PME and OASE connect via CAPE-OPEN interface

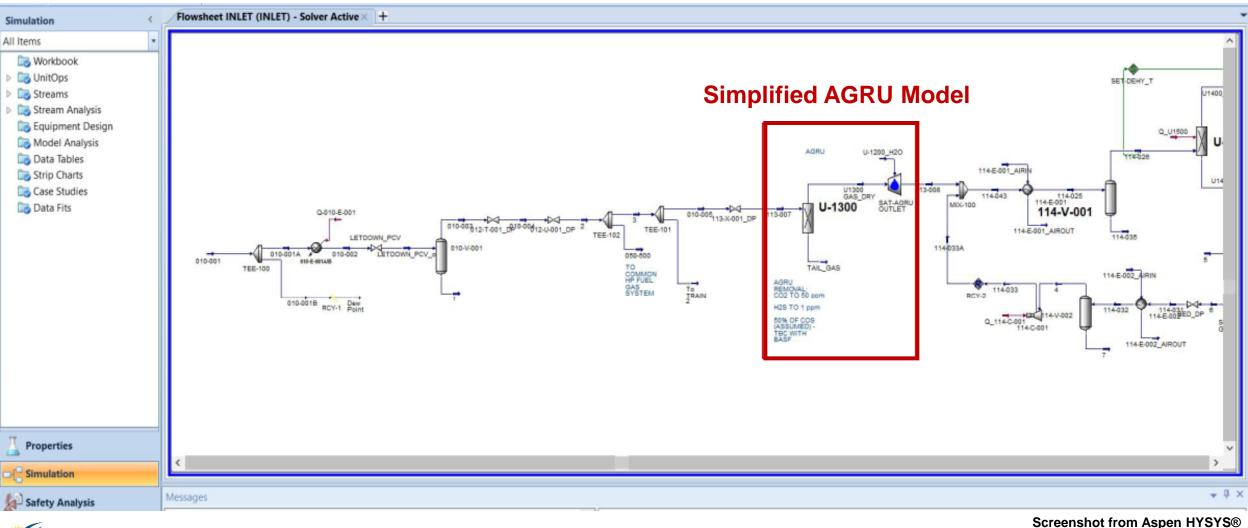






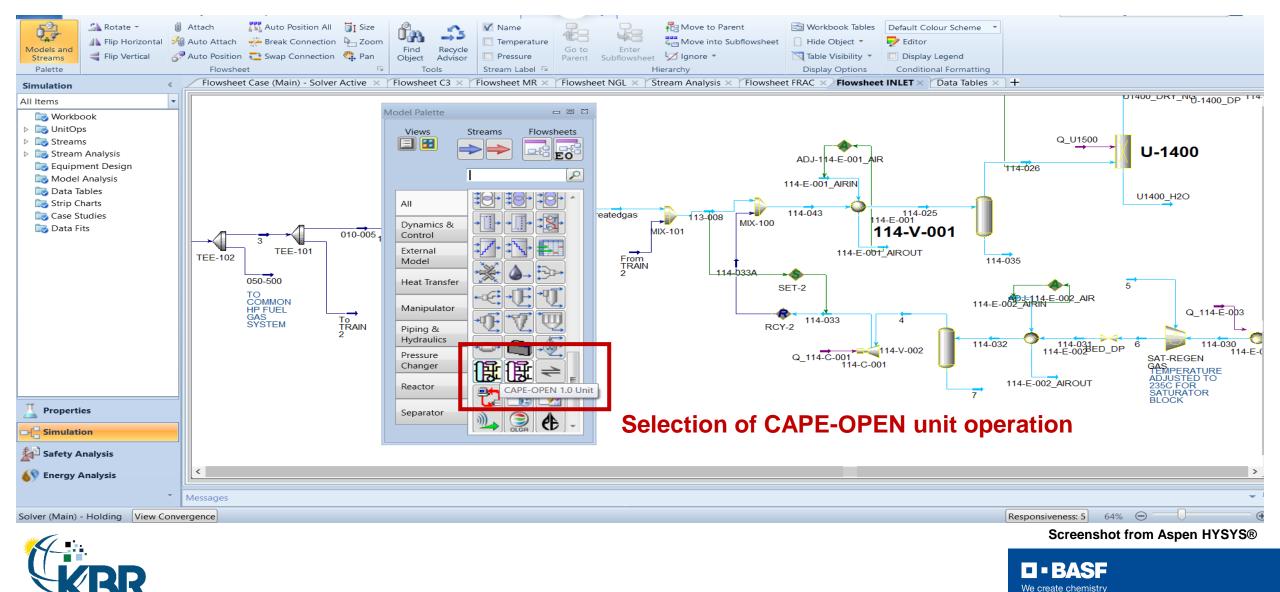
**D** • BASE

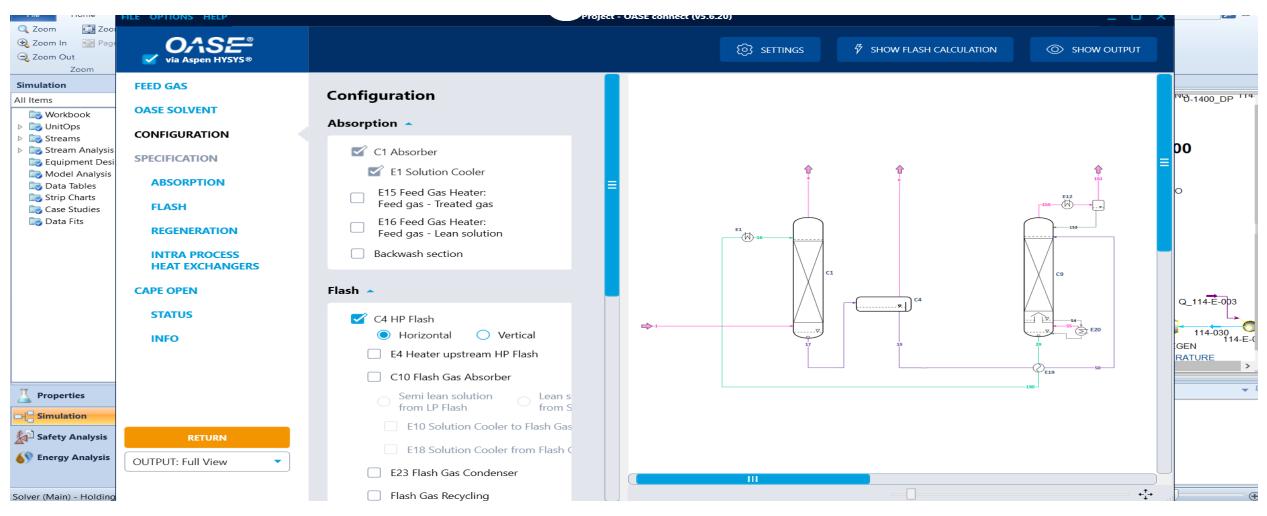
We create chemistry





**D = BASF** We create chemistry





Screenshot from Aspen HYSYS®





| Clipboard Units  | Simulation         | Solver Im                 | Summai             | les                    |              | Analysis                                       |                                     | Safety                     |                       |                                      |
|--|--------------------|---------------------------|--------------------|------------------------|--------------|--|-------------------------------------|----------------------------|-----------------------|--------------------------------------|
| Simulation   | < Flowshee         | et Case (Main) - Solver A | ctive × Flow       | sheet C3 × Flowsheet M | VIR × Flowsh | eet NGL × Stream Analys                        | is $\times$ Flowsheet FRAC $\times$ | Flowsheet INLET × Data Ta  | bles × +              |                                      |
| All Items  | •                  |                           |                    |                        |              |  |                                     |                            |                       | <u></u>                              |
| Contraction workbook                                       |                    |                           |                    |                        |              |  |                                     |                            |                       |                                      |
| 👂 📷 UnitOps  |                    |                           |                    |                        |              |  |                                     |                            |                       |                                      |
| 👂 📷 Streams  | (€ CO-100)         |                           |                    |                        | ×            |  | _                                   |                            |                       | 0.111500                             |
| Stream Analysis  | _                  | S Unit Variables Genera   |                    |                        |              |  | Acidgas                             | 3                          | ┌-�़                  | Q_U1500<br>→                         |
| Contraction Equipment Design<br>Contraction Model Analysis | -                  | reams and Material Ports  | ·                  |                        | ~            | AGRU REMOVAL:                                  | FlashGas                            | AD                         | J-114-E-001_AIR       | 1114-026                             |
| Data Tables  |                    |                           | Discritica         |                        |              | AGRU REMOVAL:<br>CO2 TO 50 ppm<br>H2S TO 1 ppm | riasiioas                           | 114 5                      |                       | 114-020                              |
| Strip Charts   | Port ID<br>FeedGas | Port type<br>Material     | Direction<br>Inlet | Material name          |              |  |                                     | 114-E-                     | -001_AIRIN            |                                      |
| Case Studies   | WaterMakeUp        | Material                  | Inlet              |                        |              |  |                                     |                            |                       | <b>→</b>                             |
| 📷 Data Fits  | TreatedGas         | Material                  | Outlet             | Treatedgas             |              |  | Treatedgas                          | 113-008 + 114-0<br>MIX-100 | 114-E-001             |                                      |
|  | AcidOffGas         | Material                  | Outlet             | Acidgas                | 01_D         | - 8  | MIX-1                               | 101                        | 114-V-001             | U                                    |
|  | Bleed              | Material                  | Outlet             | Bleed                  |              |  |                                     |                            | 114-E-001_AIROUT      |                                      |
|  | FlashGas           | Material                  | Outlet             | FlashGas               |              | CO-100   | Bleed From<br>TRAIN<br>2            |                            | 114-E-00T_AIROUT      | 114-035                              |
|  | Purge              | Material                  | Outlet             |                        |              |  | 2                                   |                            |                       |                                      |
|  | E20                | Energy                    | Outlet             |                        |              |  |                                     | SET-2                      |                       | <b>Ą</b>                             |
|  | E1                 | Energy                    | Outlet             |                        |              |  |                                     |                            |                       | ADJ=114-E-002_AIR<br>114-E-002_AIRIN |
|  | E12                | Energy                    | Outlet             |                        |              | Connecti                                       | ng the                              |                            | 14-033 4              |                                      |
|  |                    |                           |                    |                        |              |  | -                                   | RCY-2                      | 4                     |                                      |
|  |                    |                           |                    |                        |              | CAPE-OP  | <b>EN</b>                           |                            | -                     | 114-032 014-031<br>114-E-002 ED      |
|  |                    |                           |                    |                        |              |  |                                     | Q_1                        | 14-C-001<br>114-C-001 | 114-E-002 <sup>9ED</sup>             |
|  |                    |                           |                    |                        |              | unit opera                                     | ation                               |                            | 114-C-001 🥌           |                                      |
|  | F                  | eed port FeedGas is no    | tconnected         | Show U                 | hit GUI      | unit oper                                      |                                     |                            |                       | 114-E-002_AIROUT                     |
| A Properties   |                    |                           |                    |                        |              |  |                                     |                            |                       | 7                                    |
| Simulation   |                    |                           |                    |                        |              |  |                                     |                            |                       |                                      |
|  |                    |                           |                    |                        |              |  |                                     |                            |                       |                                      |
| Aralysis   |                    |                           |                    |                        |              |  |                                     |                            |                       |                                      |
| 🔊 Energy Analysis  |                    |                           |                    |                        |              |  |                                     |                            |                       | <u> </u>                             |
|  | Messages           |                           |                    |                        |              |  |                                     |                            |                       | ▼ .                                  |
| Solver (Main) - Holding                                    | ew Convergence     |                           |                    |                        |              |  |                                     |                            | Responsiveness: 5 649 | % ⊝ ──── €                           |
|  |                    |                           |                    |                        |              |  |                                     |                            |                       | ot from Aspen HYSYS®                 |
|  |                    |                           |                    |                        |              |  |                                     |                            | BASF                  |                                      |

| 🕑 i 🖬 🤊 🌾 🚍 🔤 🗉 🔻  | FILE OPTIONS HELP                | TIONS HELP New Project - OASE connect (v5.6.20) _ |               |              |          |                        |             |  |  |
|--|----------------------------------|---|---------------|--------------|----------|------------------------|-------------|--|--|
| File Home Economics  |                                  |   |               |              | SETTINGS | SHOW FLASH CALCULATION | SHOW OUTPUT |  |  |
| R Streams Streams Flip Vertical  | FEED GAS                         |   |               |              |          |                        |             |  |  |
| Simulation  All Items  | OASE SOLVENT                     |   |               |              |          |                        |             |  |  |
| PD Workbook  | CONFIGURATION                    | Save converged run as                             | :             | Open Dialog  |          |                        |             |  |  |
| <ul> <li>Image: Streams</li> <li>Image: Stream Analysis</li> <li>Image: Stream Analysis</li> <li>Image: Stream Analysis</li> </ul> | SPECIFICATION<br>ABSORPTION      | Component mapp                                    | ing           |              |          |                        |             |  |  |
| Model Analysis<br>Data Tables<br>Strip Charts  | FLASH                            | via Aspen HYSYS®                                  |               | OASE connect |          |                        |             |  |  |
| Case Studies   | REGENERATION                     | Component   | Mapping       | Component    | _        |                        |             |  |  |
| 8  | INTRA PROCESS<br>HEAT EXCHANGERS | Hydrogen  | CAS 🔹         | H2           |          |                        |             |  |  |
|  | CAPE OPEN                        | Helium  | CAS           | HE           |          |                        |             |  |  |
| ų  | STATUS                           | Nitrogen  | CAS 🔹         | N2           |          |                        |             |  |  |
|  | INFO                             | CO2   | CAS 🔹         | CO2          |          |                        |             |  |  |
| Pt Z Properties  |                                  | H2S   | CAS 🔹         | H2S          |          |                        |             |  |  |
| Simulation   |                                  | Methane   | CAS 🔹         | CH4          |          |                        |             |  |  |
| Safety Analysis  | RETURN                           | Ethane  | CAS 🔹         | С2Н6         |          |                        |             |  |  |
| -  | OUTPUT: Full View                | Ethylene  | Unspecified • | Unset        |          |                        |             |  |  |
| Solver (INLET) - Ready View Converg  |                                  |   |               |              |          |                        |             |  |  |



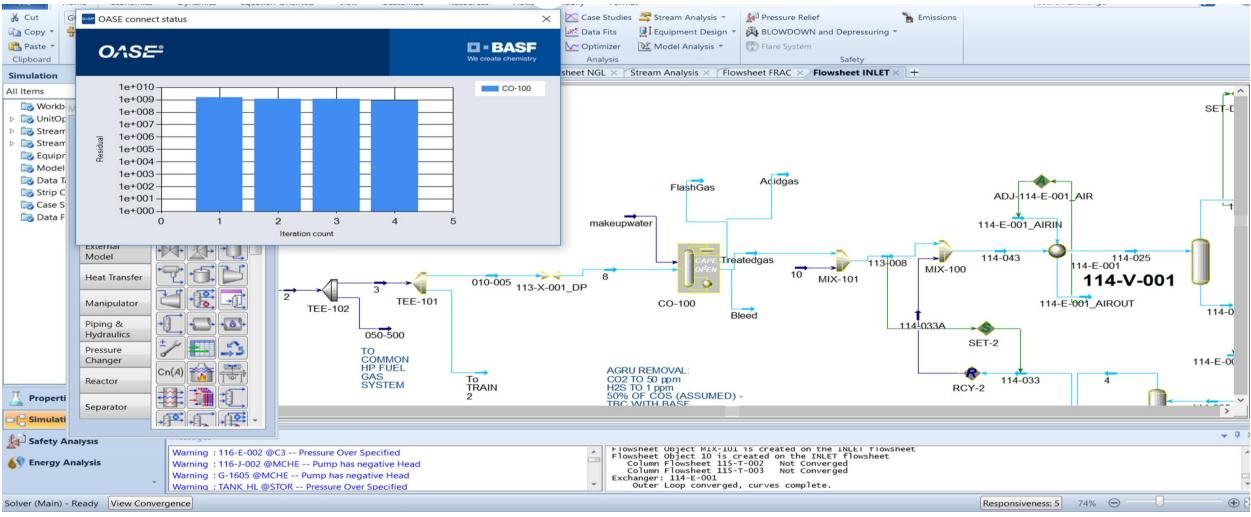
Screenshot from Aspen HYSYS®



| File Home Econo<br>Cono<br>Models and<br>Streams<br>Palette                    | FEED GAS                         | mole % (wet)        | 874901.92 Nm3/hr               | SHOW FLA  | ASH CALCULATION |       |
|--|----------------------------------|---------------------|--------------------------------|---|-----------------|-------|
| Simulation All Items   | OASE SOLVENT                     | CO2 1.9995          | H2S 3.9332E-04                 | N2 1.4997   |                 |       |
| © Workbook<br>▷ © UnitOps  | SPECIFICATION                    | CH4 90.6313         | C2H6 4.7649                    | C3H8 0.6419   |                 |       |
| <ul> <li>Streams</li> <li>Stream Analysis</li> <li>Equipment Design</li> </ul> | ABSORPTION                       | C4H10 0.1940        | i-C4H10 0.1100                 | C5H12 0.0720  |                 |       |
| lie Model Analysis<br>lie Data Tables<br>lie Strip Charts                      | REGENERATION                     | C6H14 0.0280        | C7H16 0.0130                   | C8H18 0.0070  |                 |       |
| Case Studies 🕞 Data Fits   | INTRA PROCESS<br>HEAT EXCHANGERS | С9Н20 0.0040        | C10H22 0.0020                  | CH3SH 2.2288E-04  |                 |       |
|  | CAPE OPEN                        | C2H5SH 0            | СЗН7ЅН 0                       | COS 7.4372E-04  |                 |       |
|  | STATUS                           | 02 0                | HE 0.0050                      | Benzene 0.0050  |                 | 11    |
|  |                                  | Toluene 0.0050      | Ethylbenz 5.0016E-04           | o-Xylene 3.3000E-04   |                 |       |
|  |                                  | m-Xylene 3.3000E-04 | p-Xylene 3.4000E-04            | H2O 0.0100  |                 | ~     |
|  |                                  | H2 0.0050           |                                |   |                 |       |
| 최고 Safety Analysis   | OUTPUT: Full View                | Total percentage    | - Č- <b>Tip:</b> To<br>right-c | set the total percentage to 100%,<br>lick the input field and choose "Fill to 100%" |                 | - 4 × |
| Solver (INLET) - Ready View  | Convergence                      |                     |                                |   |                 |       |



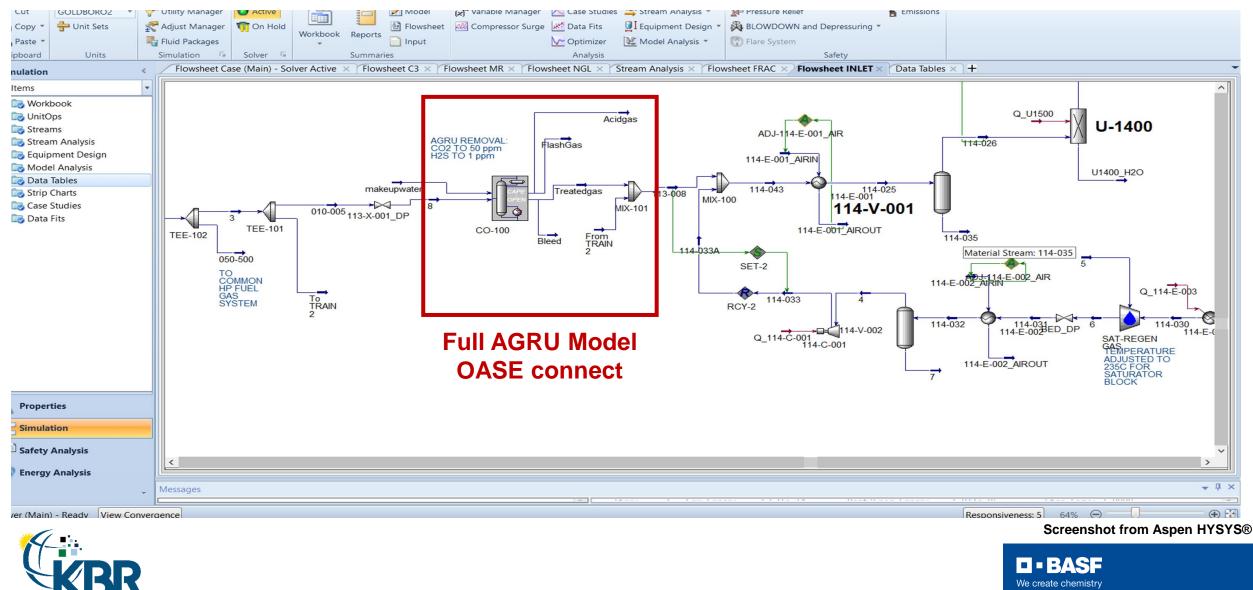
**BASF** We create chemistry





Screenshot from Aspen HYSYS®





## **Embedding OASE® connect into a Process Modeling Environment** via the CAPE-OPEN interface

**Benefits:** 



Provide a **fully closed heat and material balance** as basis for the **generation of technical datasheets** and **further equipment design** 



Changes in operating or design parameters are automatically reflected in all connected downstream engineering steps



Boosts the efficiency of collaboration in teams with a global setup



Significant savings in







