8.1 Extension for dynamic simulation

Moving from steady-state simulation to dynamic simulation
UNIT interface specification is targeted at steady-state process simulation only.

Growing need for dynamic simulation and for plugging 3rd-party modules in dynamic simulators.

Extension to current specification handled by the UNIT SIG

- Interface specification documentation written
- Prototyping:
  - IFP: UNIT operation plugs
  - INDISS: UNIT operation plugs and sockets
  - FANTOFT: UNIT operation socket
Main features

- Retain UNIT 1.0 concepts
- Add functionality to steady-state UNIT
- New concepts created
- Essentially targeted at modular sequential dynamic simulation:
  - solution strategy used in training simulators
Modular Dynamic Simulation

Unit categories:

- **Arc**: flow module without time lag
  - Valve, ShortPipeSegment, Pump, Compressor, Turbine, ShortHeatExchangerSide
  - Inlet and outlet pressures are different
  - Inlet and outlet flows are identical

- **BiArc**: flow module with pressure drop and different inlet and outlet flows
  - Long pipes

\[ \begin{align*}
F_{\text{in}} & \quad \rightarrow \quad \text{Module} \quad \rightarrow \quad F_{\text{out}} \\
P_{\text{in}} & \quad \rightarrow \quad \text{Module} \quad \rightarrow \quad P_{\text{out}}
\end{align*} \]
Modular Dynamic Simulation

Unit categories:

- **Node**: module with a small time lag
  - flow mixing points like pipe junction or header or small vessels
  - Inlet and outlet pressures are identical

- **NetworkBoundary**: battery limit for the simulation or module with a large time lag
  - distillation columns, phase separators and other large vessels
Behaviour

Dynamic simulation in a simple network

Knowing \( P_{\text{in}}(t), P'_{\text{in}}(t), P_{\text{out}}(t), T_{\text{in}}(t), T'_{\text{in}}(t) \), and every Public Unit Parameter of every UO (length, diameter, ….) what is the state of the system and its time evolution?

- Flow, pressure and temperature everywhere in the network at each moment
Dynamic simulation

Three steps in sequence

First Compute

Network Compute

Last Compute

Iterative phase

t=0

Iterative phase

(=Newton iterative variables
are node pressures)
First compute step

Compute properties that are not thermodynamically dependent

- Ex: update a valve $C_v$ according to the new opening (user input or controller), update the new limit conditions,...
Resolution (eg. Newton-based) of the node material balance \((F_1 + F_2 - F_3 = 0)\) gives \(P_{\text{calculated}}\)
Last compute step

\[ P'_{in} \rightarrow F_2 \rightarrow P_{calculated} \rightarrow F_3 \rightarrow P_{out} \]

\[ F_1 \]

\[ P_{in} \]

\[
\begin{align*}
\text{\textbf{Energy balance}} & \\
\Rightarrow \text{Update thermodynamic properties on the whole network} & \\
\text{\textbf{At the end of this stage the system has been calculated at time } t} & 
\end{align*}
\]
Dynamic interfaces

NetworkBoundaries

- Do not support any specific interfaces but ICapeDynamicUnit.

Nodes

- Specific unit operations characterised by:
  - Inlet and outlet pressure are identical
  - Hold up.
- Implement two interfaces: ICapeDynamicUnit and ICapeNodeDynamicUnit
Dynamic interfaces

- **Arcs**
  - Specific unit operations characterised by:
    - Pressure drop
  - Implement two interfaces: ICapeDynamicUnit and ICapeArcDynamicUnit

- **BiArcs**
  - Specific unit operations characterised by:
    - Pressure drop
    - Inlet and outlet flows are different
  - Implement two interfaces: ICapeDynamicUnit and ICapeBiArcDynamicUnit
Implementations: INDISS, IFP, D-SPICE
Specification document

- Draft has been prepared
- Available from UNIT SIG and CTO
- Prototyping:
  - Already done by IFP and RSI
  - To be confirmed by Fantoft
- Comments are welcome
Perspectives

Use CO UNIT in mixed EO and SM solution strategies

- Aspen Plus implements parts (socket) of the SOLVER interface specification:
  - Equation Set Object (ESO) and Matrix
- Aspen Plus Mixer example implements ESO interface
- In search for a UNIT plug from a 3rd party implementing ESO interface

Would enable to use EO solution strategy in Aspen Plus with a CAPE-OPEN Unit

Maybe soon gPROMS will provide a UNIT socket with ESO interface to plug Aspen Plus Mixer