Mathematical concepts behind system composition

Modelon Innovate 2024 – Day 2

Team Modelon

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Why this session matters?

- What happens mathematically when components are dragged to the canvas and connected?
- A look behind the scene…
- Connect fluid components → Robust and efficient system models

Overview

- Fluid properties (State)
- Conservation laws
- Constitutive relations
- Workshop 1
- Connecting fluid components for robust & efficient system models
- Workshop 2

→ Shared workspace: **Innovate-MathematicalConcepts**

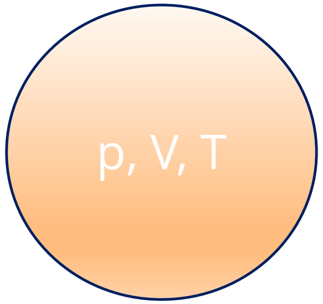
FLUID PROPERTIES (STATE)

Minimal representation

Compute all equilibrium properties from a small set of variables and equations!

– Set of variables = **State**

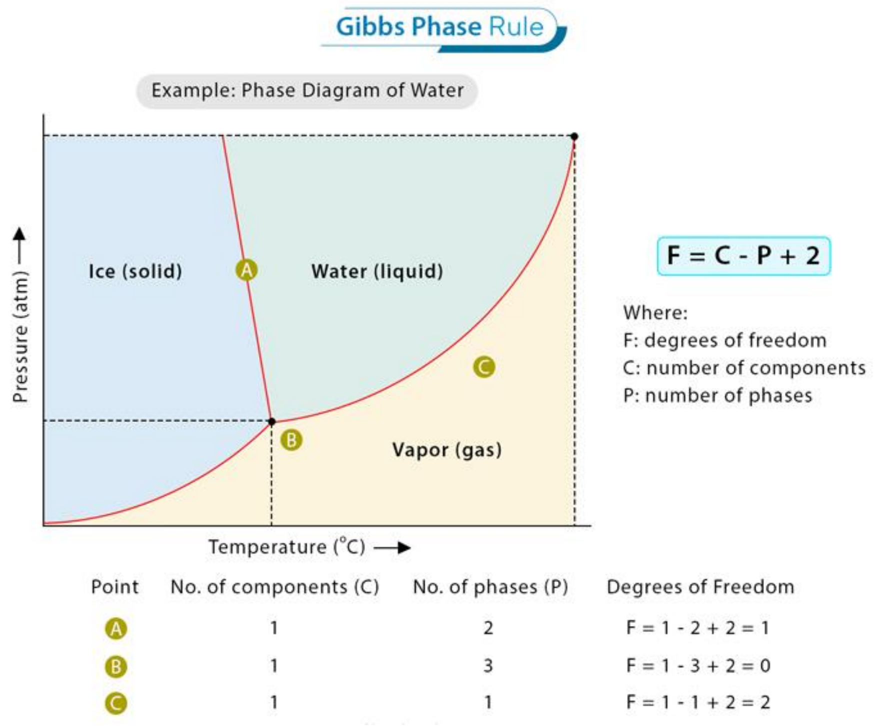
– Set of equations = **E**quations **O**f **S**tate (EOS)



Fluid state

Requirements

- Independent of history
- Sufficient to derive all properties
- Works for all phases and mixtures (see Gibbs' phase rule)



picture courtesy of chemistrylearner.com

- Two-phase pure fluid
  - One **extensive**
  - Two *intensive*
  - Ex: **V**, *p, h*
- Single-phase mixture
  - One **extensive**
  - Three *intensive*
  - Ex: **V**, *p, T, X*

State and derived properties

- In addition to thermodynamic properties that can be used to describe the state, other properties are relevant to describe how materials react to changes of states, e.g.,
  - Specific heat capacities, compressibility…

$$c_p = \left.\frac{\partial h}{\partial T}\right|_p \qquad \kappa = \left.\frac{1}{v}\frac{\partial v}{\partial p}\right|_T$$

  - Transport properties: viscosity, conductivity, surface tension…

- Medium functions are used to describe the EOS and other property calculations

CONSERVATION LAWS

Conservation laws

- Conserved quantity
  - Mass
  - Energy
  - Momentum
- Global balance in volume

$$Rate\ of\ change = Flow_{in} - Flow_{out} + source$$

- Static or dynamic

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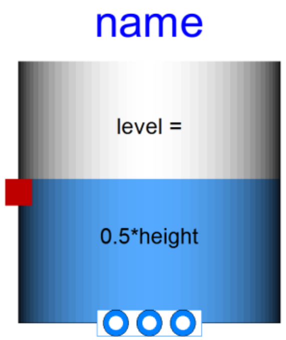
Mass balance, open

- System = control volume

$$\frac{dm_{cv}}{dt} = \dot{m}_{in} + \dot{m}_{out}$$

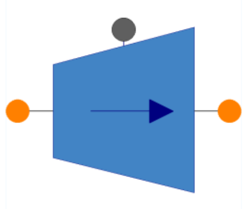
$$m_{cv} = \rho V_{cv}$$

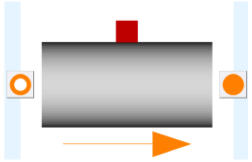


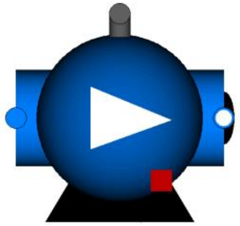
- Modelica: positive flow into the volume
- Incompressible fluid or small volume: no accumulation

$$\frac{dm_{cv}}{dt} = 0 \Rightarrow \dot{m}_{in} + \dot{m}_{out} = 0$$

Energy balance, open







$$\frac{dE}{dt} = \dot{m}_{in} \cdot e_{in} + \dot{m}_{out} \cdot e_{out} + \dot{Q} + \dot{W}$$

$$\dot{W} = \dot{W}_{shaft} + \dot{W}_{flow}$$

$$\dot{W}_{flow} = pv\dot{m}$$

$$h = u + pv \qquad e = u + {c^2}/{2} + g \cdot z$$

$$\frac{dE}{dt} = \dot{m}_{in} \cdot h_{in} + \dot{m}_{out} \cdot h_{out} + \dot{Q} + \dot{W}_{shaft}$$

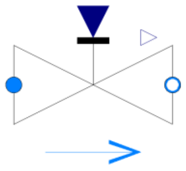
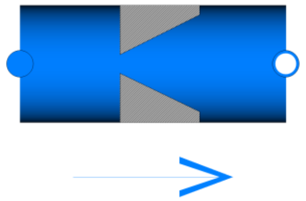
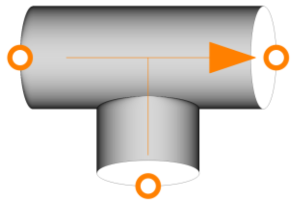
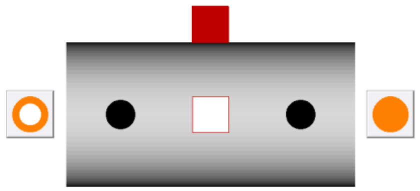
$e \approx u$, natural dynamical state
h, natural choice at ports

Momentum balance

$$\frac{\partial q}{\partial t} + v\frac{\partial q}{\partial x} = -\frac{A}{\rho}\frac{\partial p}{\partial x} + f(q)$$

- Assuming pressure and friction forces
- Flow driven by pressure difference
- Fast dynamics
- Steady state, low Mach number:

$$\frac{A}{\rho}\frac{\partial p}{\partial x} = f(q)$$

CONSTITUTIVE RELATIONS

Constitutive relations

- Pressure drop $\Delta p_f = f(Re, l, d)\frac{l}{d}\frac{\dot{m}}{\rho A}$

- Heat transfer $\dot{q} = h(Re, Pr, \dot{m}) A \Delta T$
  - Conductive
  - Convective
  - Radiative

- Component specific characteristics
  - Performance maps or functions for turbines, compressors, etc.

Workshop 1

In this workshop you will identify the balance equations in:

- Modelon.ThermoFluid.Volumes.MultiportVolume
- Modelon.ThermoFluid.FlowResistances.FrictionLoss

What can you say about the dynamics of each of the balance equations?

Look in particular for the difference between energy and mass balance in the volume component on one hand and the momentum balance in the flow component.

What is the difference between their implementation? Where are the states located?

Solution

For (1.) you should have been able to explicitly determine the mass as well as energy balance.

For (2.) you should have been able to determine the momentum balance (implemented through a function), the mass and energy balance are accounted for as the inlet and outlet mass flow and enthalpy are set equal at both ports.

The energy and mass balance contain a time derivative and imply that there will be states during the simulation. The energy and mass balance are considered slow: energy and mass might accumulate or be drained over time. The momentum balance does not have a derivative and the friction component does therefore not contain a state. Changes occur instantaneously. The momentum balance is an algebraic equation.

CONNECTING FLUID COMPONENTS

Types of fluid component model

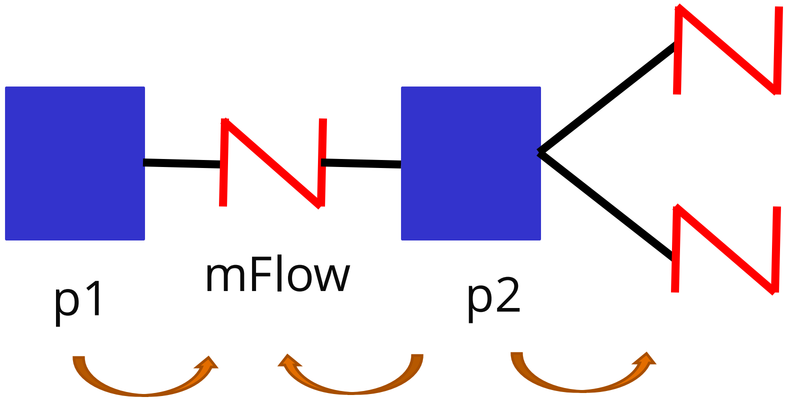
- **Volume model:** (tanks, HXs, reactors etc.)
  - Implementation of mass and energy balances
  - Sets enthalpy and pressure
  - Friction is negligible

$$\frac{dM}{dt} = \sum \dot{m}_i$$

$$\frac{dU}{dt} = \sum \dot{m}_i h_i + \sum q_j$$

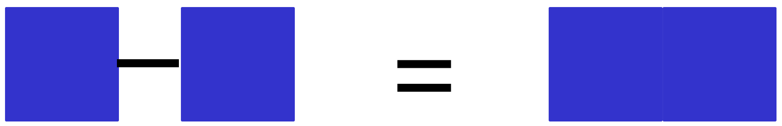
- Flow type model: (valves, compressors, etc.)
  - Implementation of momentum balance (and mass balance)
  - Sets mass flow rate
  - Friction is the characteristic feature

$$\Delta p_f = f(\dot{m}, \mathrm{Re}, \rho, l, d)$$



Connecting fluid components

- Direct coupling of volume type models:

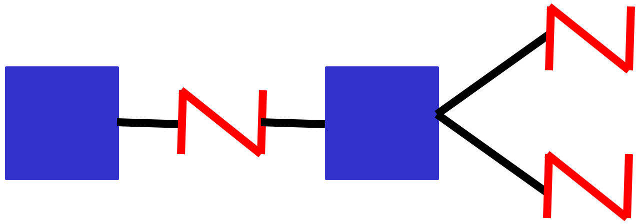


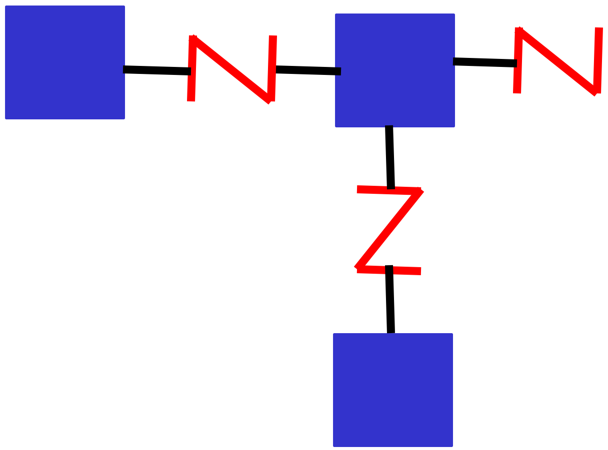
  - Constraints between differentiated variables (pressures equal) structural index 2 DAE.
  - Not recommended, except for very simple property models.
  - Interpretation of flow variables between volumes difficult, very unusual thinking in component-oriented system modeling
- Direct coupling of flow type models:

- Non-linear systems of equations for algebraic mass - and energy balances between flow models.
  - Can be problematic numerically, not recommended in most cases.

Connecting fluid components: recommendation

- Recommended way of modeling:



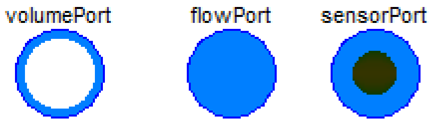


Always alternate
flow and volume models!

- Be aware of what the important system elements for storage of mass and energy are.
- Be prepared to neglect small volumes or lump several volumes at one place.
- Try to always alternate *volume* type and *flow* type models.
- Resulting structure: no non-linear systems are created by connecting components, only local ones exist inside components, if proper states are chosen.

Connecting fluid components: connector icon

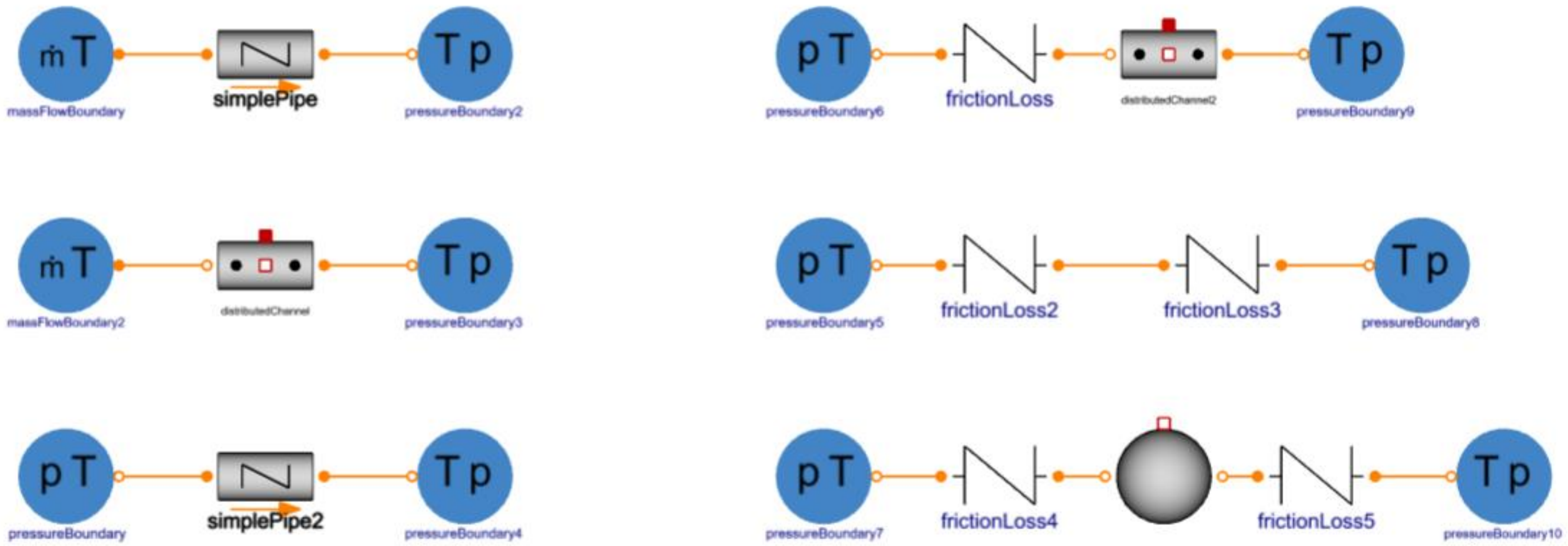
- 3 types of connector icons in Modelon thermo-fluid libraries



  - volumePort indicates pressure state
  - flowPort indicates pressure correlation

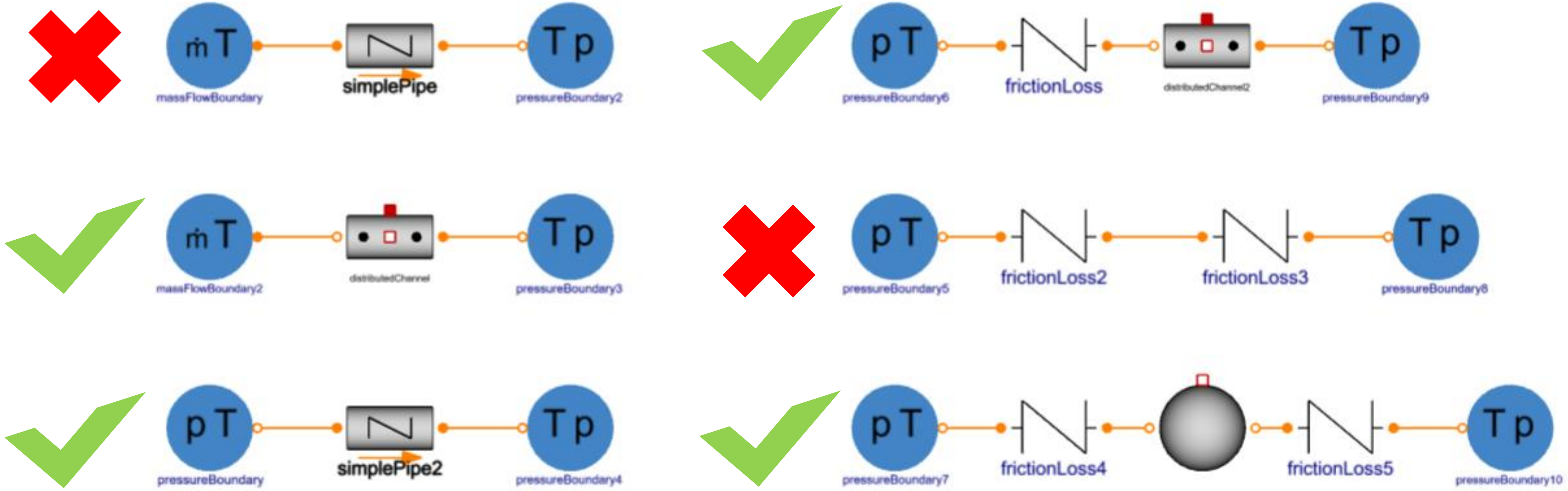
- Connection rules to support fast and robust simulation code
  - volumePort - flowPort - volumePort
  - No connection rules for sensorPort

Workshop 2



Select the right configuration for connecting fluid components in the above examples.

Solution



Violation may lead to over-specified initialization problems or/and less robust simulation code

Questions?

References:

- https://help.modelon.com/latest/training/Day2/Equationbased_Modeling/
- https://help.modelon.com/latest/training/Day3/From_ModelicaModel_To_SimulationModel_Compiler_and_Solver_insights/

Modelon Impact

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