Project – Introduction to Part 3

Lecture ME 454

Modeling and Optimization of Energy Systems

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Project – Part 3

Provide decision support to EPFL to choose a working fluid for the novel centralized heating system composed of a two-stage HP with maximum capacity of 6 MW based on environmental and economic characteristics.

Tasks:

1. Build a thermodynamic model of the two-stage HP in the process simulation software Belsim VALI
2. Use measurement data for performing Degrees of Freedom (DoF) and data reconciliation analyses
3. Use the results of the data reconciliation to evaluate the thermodynamic and economic performances of the system

Modelling of a simple heat pump – Optional

Tutorials on SwitchTube

1. Vali Tutorial
   i. Opening Vali
   ii. Creating a first PFD
   iii. Defining Thermods

2. Heat pump compressions
   i. Creating streams
      - Material
      - Mechanical
   - Defining units
      - Compressor

3. DoF analysis and running

4. Heat pump remaining steps
   i. Defining units
      - Heat exchanger
      - Valves
   ii. Defining streams
      - Thermal

5. Closing loops
   i. Defining units
      - Cutval
   ii. Debugging
      - Error reporting
      - DOF reporting
   iii. Running

Modelling of a two-stage HP – Flowsheet

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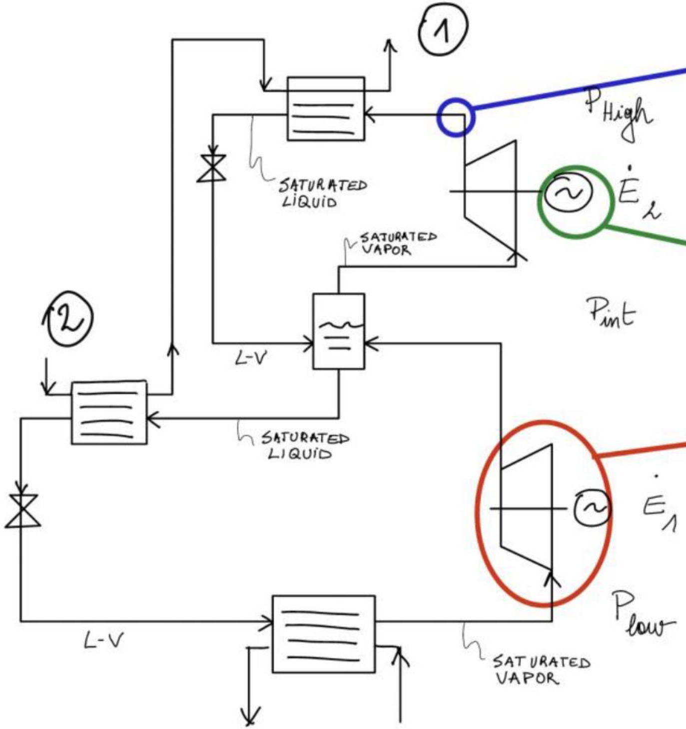

Flows interconnecting units
- Flowrate
- Thermodynamic State
  T, P, X

Power

Process unit : converting flows
- Size
- Type
- Conversion of mass and energy

Belsim VALI

Flowsheeting and data reconciliation tool:

- Equation-based data validation and reconciliation (DVR) software, respecting energy and mass balances
- Uses information redundancy and conservation laws to correct measurements and convert them into accurate and reliable information
- Used in upstream, refinery, petrochemical and chemical plants as well as power plants, including nuclear power stations

Modelling of a two-stage HP – Belsim VALI

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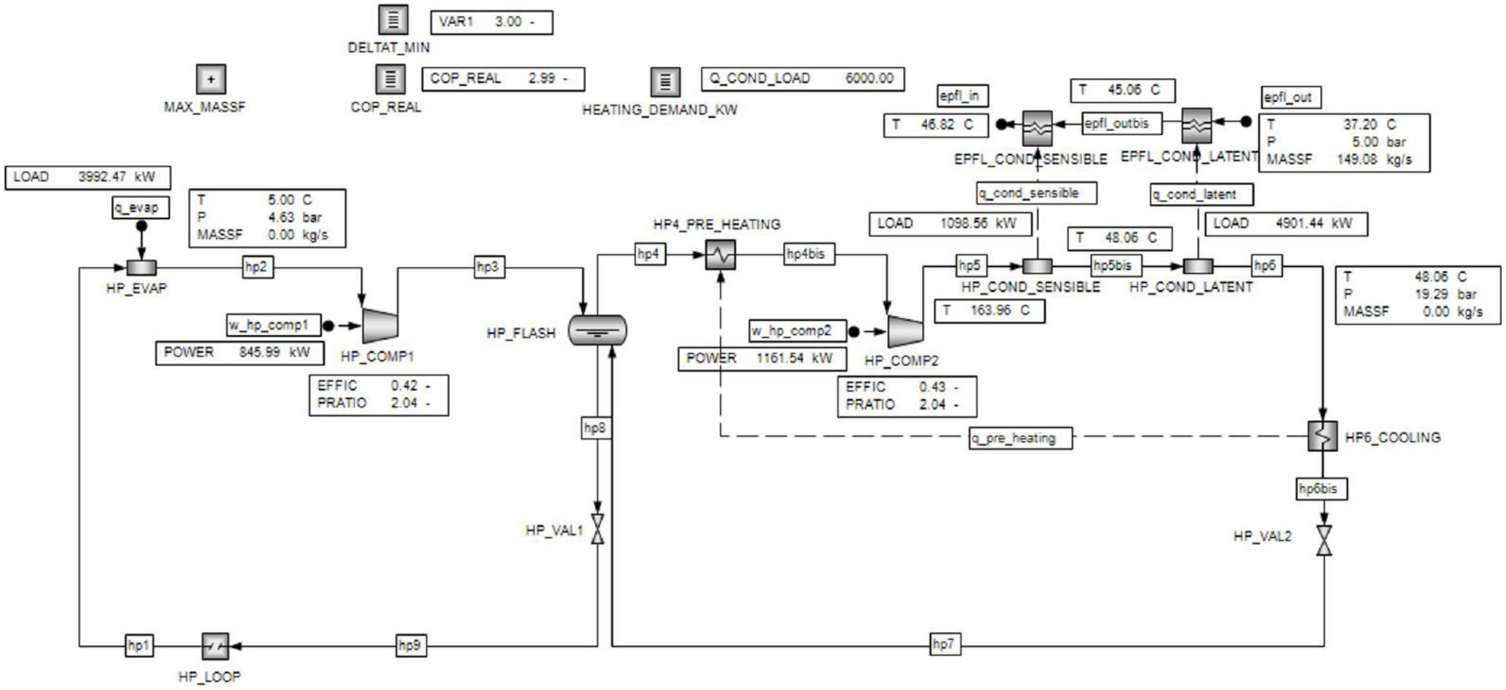


Working Fluids

ASHRAE number	Name	Group	GWP	ODP	Lifetime τ [yr]	Safety Group
R-290	Propane	HC	3.3	0	12	A3
R-600	Butane	HC	4	0	12	A3
R-600a	Isobutane	HC	3	0	12	A3
R-717	Ammonia	N	0	0	0.02	B2L
R-1234yf	Tetrafluoropropene	HFO	4	0	0.03	A2L
R-1234ze	Tetrafluoropropene	HFO	6	0	0.05	A2L
R-1270	Propylene	HO	1.8	0	12	A3
R-12	*Dichlorodifluoromethane*	*CFC*	*10'900*	*1*	*100*	*A1*

- All the steps described next need to be carried out for the R-290 and another working fluid of choice

→ Remember to use the corresponding Vali model!

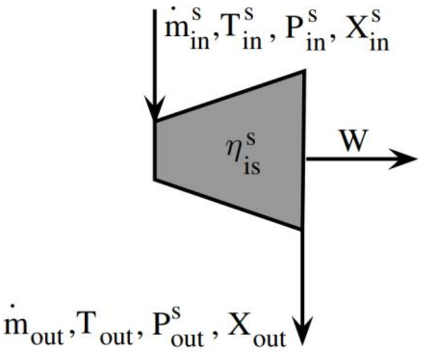
- **Justify your choice considering thermophysical and economic features, safety concerns, environmental impact, and other properties you judge relevant**

DoF Analysis – Flowsheet

- Degrees of Freedom: $n_{DoF} = n_{variables} - n_{equations}$

e.g. Compressor unit

- $n_{variables} = 14$
- $n_{equations} = 9$
  - Mass balance - $\dot{m}_{out} - \dot{m}_{in}^{s} = 0$
  - Enthalpy of the input - $h_{in} - h(T_{in}^{s}, P_{in}^{s}, X_{in}^{s}) = 0$
  - Entropy of the input - $s_{in} - s(T_{in}^{s}, P_{in}^{s}, X_{in}^{s}) = 0$
  - …
- $n_{DoF} = 5$



- **The DoF analysis needs to be carried out for the process flowsheet of the whole two−stage heat pump**

DoF Analysis – Excel Sheet

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DOF.csv

Tag Name	Physical Unit	Option 1	Option 2	Option 3	Option 4	Option 5
HP_COMP1_EFFIC	-	OFF	CST	CST	OFF	CST
HP_COMP1_PRATIO	-	CST	OFF	CST	OFF	OFF
HP_FLASH_DP	bar	OFF	CST	OFF	CST	CST
HP_COMP2_EFFIC	-	CST	CST	CST	OFF	CST
HP_COND_LATENT_DP	bar	OFF	OFF	CST	CST	OFF
HP_EVAP_DP	bar	CST	OFF	CST	CST	OFF
COP_REAL	-	OFF	OFF	OFF	OFF	CST

1. Perform the DoF analysis of the model of the two-stage heat pump
2. Evaluate which of the 5 options in the Excel file is the right one:
   - **OFF** = feeding the model with a constant value of these variables would lead to overspecification
   - **CST** = specifications to be provided to solve the model
3. Open one of the R-XXX_empty.bls file in Vali and activate the necessary TAGS

   → Do not change any values but just change the accuracy tab from OFF to CST
4. Run the model and hope for convergence

- **Don’t forget to activate the Edit Mode!**

DoF Analysis – Belsim VALI

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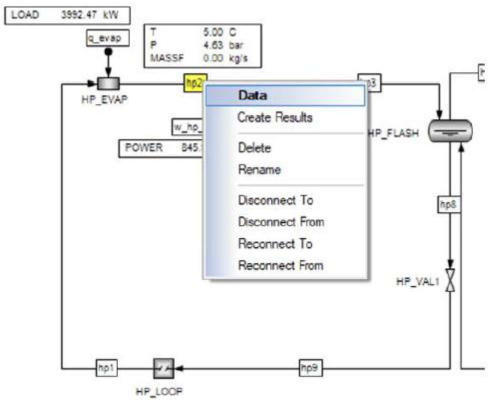

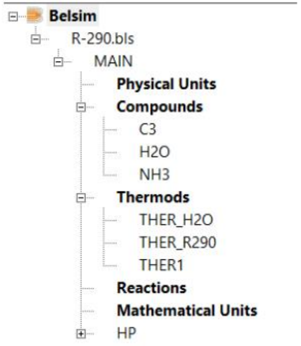

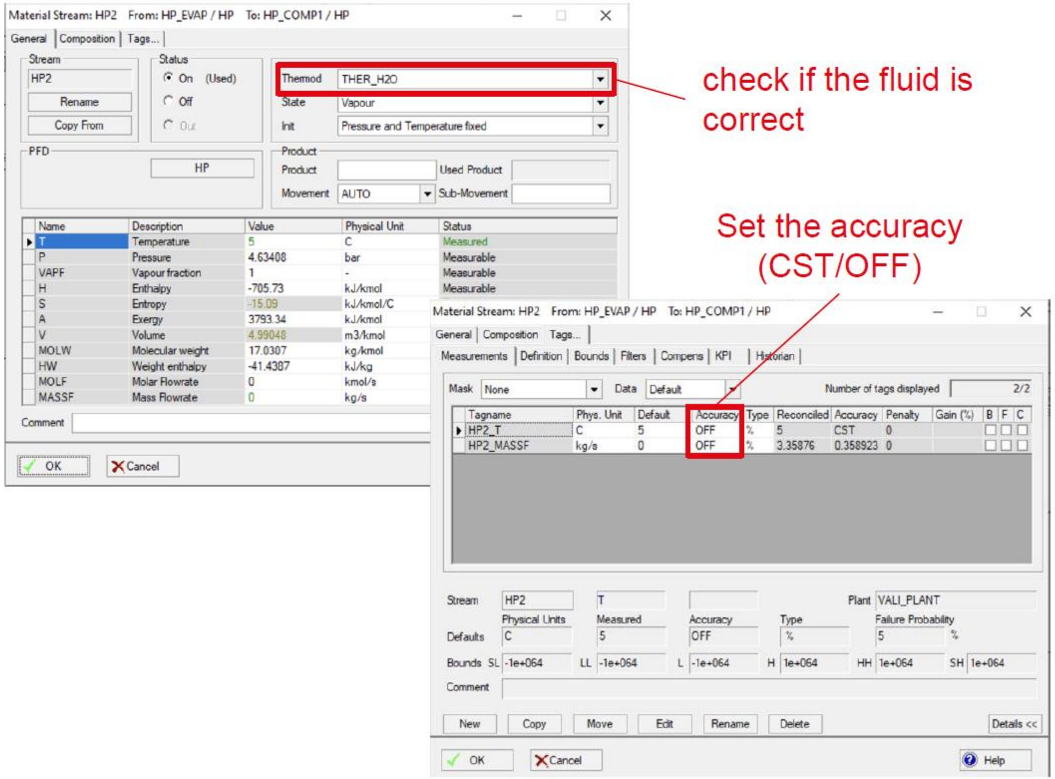

check if the fluid is correct

Set the accuracy (CST/OFF)

Data reconciliation

- *Measured data contains inconsistencies*:
  - **Random errors** → sensor location, plant instabilities, measurements taken at different times, etc.
  - **Systematic errors** → sensor calibration, measurement bias, intrinsic sensor precision, etc.

→ Data reconciliation ensures that there are no violations of mass and energy conservation laws

- **Data reconciliation relies on measurement redundancy**

  → The measured values of the variables that are not set as specifications for the resolution of the model are redundant

- **The data reconciliation problem statement minimizes the error between the measured values and the validated one**

  → Validated values solve the system model equations

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Data reconciliation – Measurements

R-290_LT_1.txt

```
COP_REAL 3.56768567878831 OFF -
DELTAT_MIN_VAR1 3.06964499386959 CST -
EPFL_IN_P 4.90108202595729 -0.1 bar
EPFL_IN_T 39.5065216193497 0.8 C
EPFL_OUT_MASSF 165.200133901951 -0.25 kg/s
EPFL_OUT_P 5.23774053831585 -0.1 bar
EPFL_OUT_T 30.371203187654 0.8 C
EPFL_OUTBIS_P 4.85457838850562 -0.1 bar
EPFL_OUTBIS_T 39.2761806539843 0.8 C
HP_COMP1_EFFIC 0.438351 OFF -
HP_COMP1_PRATIO 1.84759478339323 OFF -
HP_COMP2_EFFIC 0.427407352518534 OFF -
HP1_T 1.97005686815828 0.8 C
HP2_MASSF 3.07024638802827 -0.25 kg/s
HP2_T 5.20112206588965 0.8 C
HP5_T 132.088442522007 0.8 C
HP5BIS_T 40.1542407296763 0.8 C
HP6_MASSF 3.80180020682021 -0.25 kg/s
HP6_T 41.8523397444798 0.8 C
MAX_MASSF_HP2 11.5304884748294 0.5 -
MAX_MASSF_HP6 12.7425721083489 0.5 -
Q_COND_LATENT_LOAD 4466.64198678494 -0.5 kW
Q_COND_LOAD 5239.04822427638 CST -
Q_COND
Q_EVAP
W_HP_C
W_HP_C
ARCHIV
DATA T
DATA
```

For 7 working fluids
For 6-11 periods
For 2 temperature levels

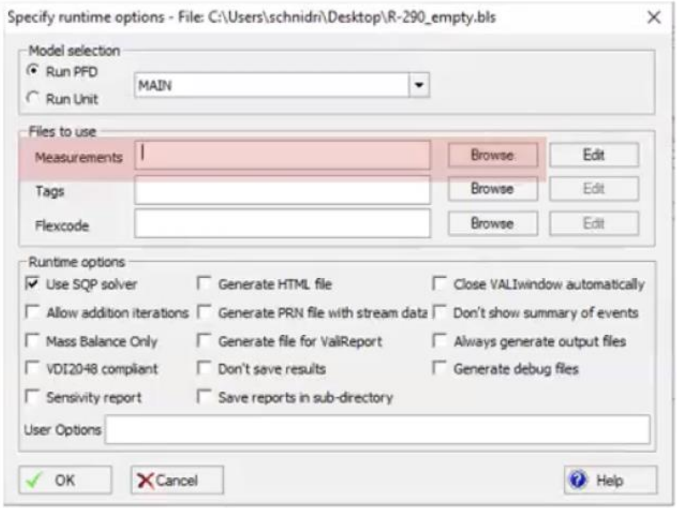
Tags	Values		Units
COP_REAL	3.567685679	OFF	-
DELTAT_MIN_VAR1	3.069644994	CST	-
EPFL_IN_P	4.901082026	-0.1	bar
EPFL_IN_T	39.50652162	0.8	C
EPFL_OUT_MASSF	165.2001339	-0.25	kg/s
EPFL_OUT_P	5.237740538	-0.1	bar
EPFL_OUT_T	30.37120319	0.8	C
EPFL_OUTBIS_P	4.854578389	-0.1	bar
EPFL_OUTBIS_T	39.27618065	0.8	C
HP_COMP1_EFFIC	0.438351	OFF	-
HP_COMP1_PRATIO	1.847594783	OFF	-
HP_COMP2_EFFIC	0.427407353	OFF	-
HP1_T	1.970056868	0.8	C
HP2_MASSF	3.070246388	-0.25	kg/s
HP2_T	5.201122066	0.8	C
HP5_T	132.0884425	0.8	C
HP5BIS_T	40.15424073	0.8	C
HP6_MASSF	3.801800207	-0.25	kg/s
HP6_T	41.85233974	0.8	C
MAX_MASSF_HP2	11.53048847	0.5	-
MAX_MASSF_HP6	12.74257211	0.5	-
Q_COND_LATENT_LOAD	4466.641987	-0.5	kW
Q_COND_LOAD	5239.048224	CST	-
Q_COND_SENSIBLE_LOAD	730.7277	-0.5	kW
Q_EVAP_LOAD	3590.426987	-0.5	kW
W_HP_COMP1_POWER	635.1348379	-0.5	kW
W_HP_COMP2_POWER	801.2989638	-0.5	kW
ARCHIVE -T Reconciled/reconc_R-290_LT_1.txt			
DATA TAG			
DATA			

Data reconciliation – Belsim Vali

With the calibrated model:

1. Upload the measurement file
2. Run the model to perform data reconciliation

→ Make sure to have a folder named "Reconciled" in the same folder as your Vali model!



a. **If converged:** you can proceed with next measurement

b. **If not converged:** you should re-run the model without measurements, then re-run it with the previous measurements, load the results and finally re-run with the current measurement file

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Data reconciliation – Results

- The output file is generated if Vali has converged to a feasible solution

→ **It includes both measured and reconciled values**

reconc_r-290_It_1.txt

```
HP_COMP1_EFFIC  0.438351    -.100000E+21    0.423483    -.883089    -
HP_COMP1_PRATIO 1.75565 -.100000E+21    1.87260 -.548547    -
HP_FLASH_DP 0.00000 0.00000 0.00000 0.00000 bar
HP_COMP2_EFFIC  0.430301    -.100000E+21    0.449755    -.984102    -
HP_COND_LATENT_DP   0.00000 0.00000 0.00000 0.00000 bar
HP_EVAP_DP  0.00000 0.00000 0.00000 0.00000 bar
COP_REAL    3.73251 -.100000E+21    3.47606 -.238130    -
HP_COND_SENSIBLE_DP 0.00000 0.00000 0.00000 0.00000 bar
EPFL_COND_SENSIBLE_DP1  0.00000 0.00000 0.00000 0.100000E+21    bar
EPFL_COND_LATENT_DP1    0.00000 0.00000 0.00000 0.100000E+21    bar
Q_COND_LOAD 5223.69 0.00000 5223.69 0.00000 -
DELTAT_MIN_VAR1 2.97675 0.00000 2.97675 0.00000 -
MAX_MASSF_HP2   11.6389 0.500000    12.4538 0.329711    -
MAX_MASSF_HP6   12.9881 0.500000    12.7812 0.336194    -
HP2_T   4.76966 0.800000    3.16273 0.342896    C
HP2_MASSF   2.98959 -.250000    3.08067 -.110648    kg/s
W_HP_COMP1_POWER    652.884 -.500000    663.321 -.439678    kW
W_HP_COMP2_POWER    839.883 -.500000    839.442 -.279404    kW
HP5_T   127.247 0.800000    133.986 0.390448    C
HP5BIS_T    40.1457 0.800000    39.1868 0.291387    C
HP6_T   42.2654 0.800000    39.1868 0.291401    C
HP6_MASSF   3.78124 -.250000    3.75418 -.851219E-01    kg/s
Q_COND_LATENT_LOAD  4312.18 -.500000    4439.68 -.534480E-01    kW
HP1_T   1.96268 0.800000    0.162730    0.343093    C
Q_EVAP_LOAD 3779.42 -.500000    3720.93 -.966408E-01    kW
Q_COND_SENSIBLE_LOAD    787.213 -.500000    784.009 -.302665    kW
EPFL_OUTBIS_T   37.4638 0.800000    36.2101 0.291401    C
EPFL_OUTBIS_P   5.08031 -.100000    5.08031 -.100000    bar
EPFL_IN_T   38.4135 0.800000    37.2873 0.291692    C
EPFL_IN_P   5.12703 -.100000    5.12703 -.100000    bar
EPFL_OUT_T  30.6327 0.800000    30.1158 0.291099    C
EPFL_OUT_P  4.99046 -.100000    4.99046 -.100000    bar
EPFL_OUT_MASSF  173.386 -.250000    173.390 -.249953    kg/s
HP2_SMOL    1.00000 0.100000E+21    -14.7569    0.627199E-01    kJ/kmol/C
HP4BIS_SMOL 1.00000 0.100000E+21    -16.4407    0.528417E-01    kJ/kmol/C
```

Tags	Measured value	Measured accuracy	Reconciled value	Reconciled accuracy	Units
HP_COMP1_EFFIC	0.438351	-1.00E+20	0.423483	-0.883089	-
HP_COMP1_PRATIO	1.75565	-1.00E+20	1.8726	-0.548547	-
HP_FLASH_DP	0	0.00E+00	0	0	bar
HP_COMP2_EFFIC	0.430301	-1.00E+20	0.449755	-0.984102	-
HP_COND_LATENT_DP	0	0.00E+00	0	0	bar
HP_EVAP_DP	0	0.00E+00	0	0	bar
COP_REAL	3.73251	-1.00E+20	3.47606	-0.23813	-
HP_COND_SENSIBLE_DP	0	0.00E+00	0	0	bar
EPFL_COND_SENSIBLE_DP1	0	0.00E+00	0	1E+20	bar
EPFL_COND_LATENT_DP1	0	0.00E+00	0	1E+20	bar

Performance evaluation – Thermodynamics

<u>*Using the reconciled data:*</u>

1. Derive a polynomial function of the Carnot factor as a function of the ambient temperature for both stages of the heat pump

- $C^*_{Carnot}(t) = a \cdot T^2_{amb} - b \cdot T_{amb} + c$

2. Minimize the mean square error between the Carnot factor calculated with the given operating conditions and the Carnot factor calculated with the polynomial function over all measurement sets

- $C_{Carnot}(t) = \frac{Q_{cond}(t)}{W_{tot}(t)} \cdot \frac{T_{cond}(t) - T_{evap}(t)}{T_{cond}(t)}$
- $\min\limits_{a,b,c} \sum_t \left(C^*_{Carnot}(t) - C_{Carnot}(t)\right)^2$

3. Calculate the Carnot factor for the temperatures of the clusters and plot the Carnot factor vs ambient temperature

Performance evaluation – Economics

Using the reconciled data:

1. Size the heat exchangers and compressors for the worst case, i.e. highest heat demand, present in the measurement set

2. Calculate the specific capital cost of the heat pump considering compressors and heat exchangers

- **Use reconciled data for different working fluids to compare the thermodynamic and economic performances of the system in each case**

Deliverables – Part 3

For the different working fluids:

- Size of the heat exchangers and compressors
- Total cost of the system including the investment cost of the heat exchangers and compressors

→ **Provide decision support to EPFL to choose the working fluid for the two-stage HP**

- Unit cost of the system per kW of heat pump capacity installed
- Carnot factor as a polynomial function of the ambient temperature T_{ext}

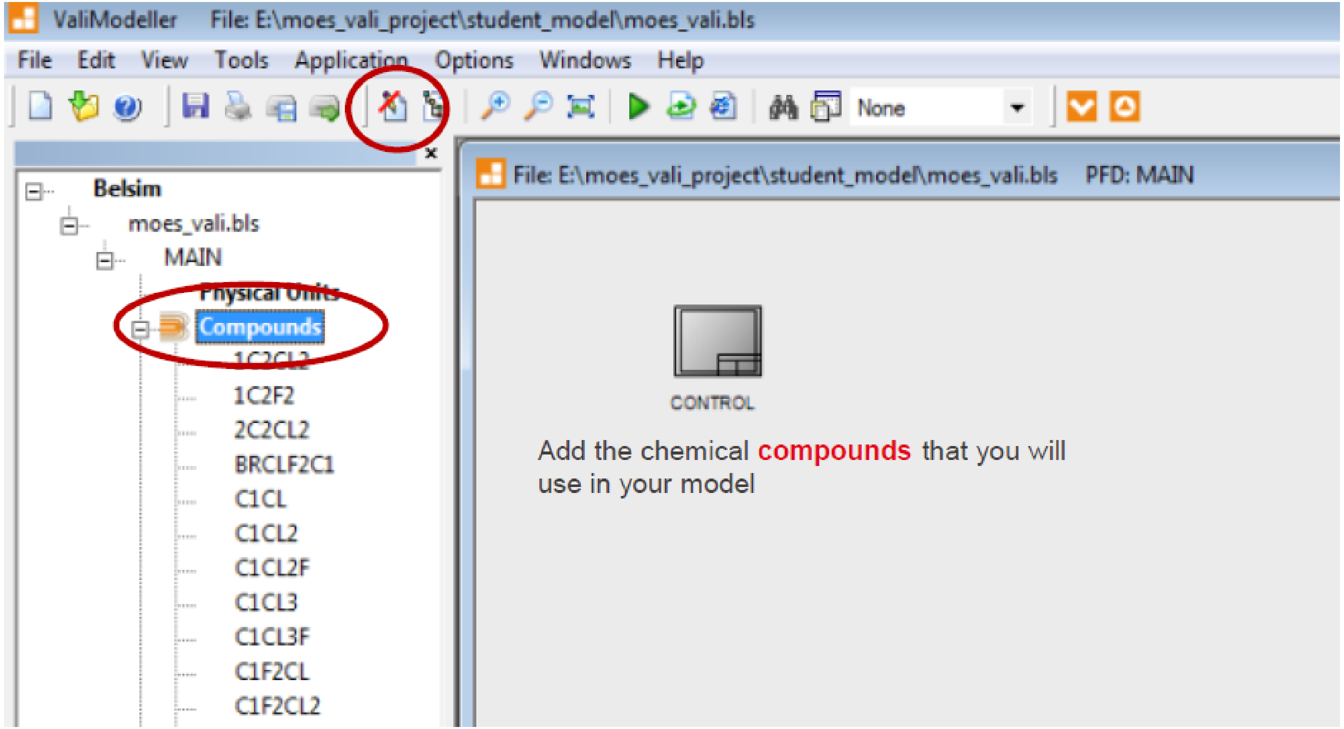
→ **Information to be used in Part 4**

Appendix – Belsim VALI

EPFL

Vali modelling basics

First turn editing on

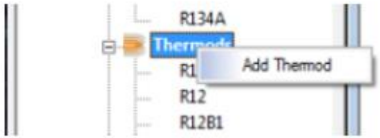


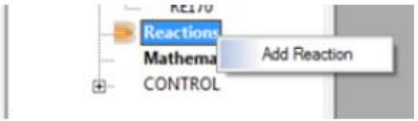
Add the chemical compounds that you will use in your model

Vali modelling basics

Add your **thermods**:

- Thermods might include only 1 compound as well as they can be a mixture of several compounds
- You must define the required compounds before being able to define the thermods



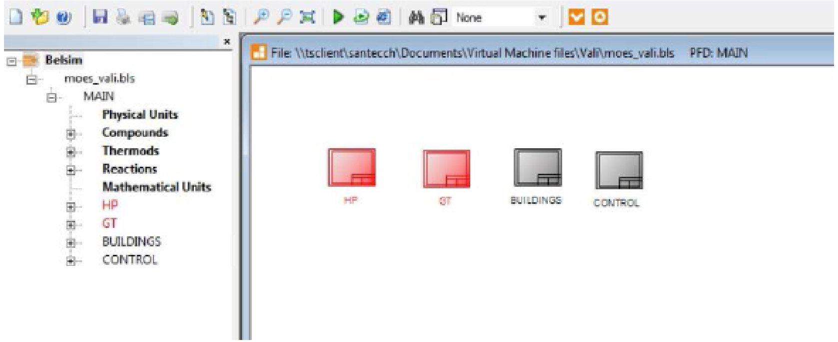


Add your chemical **reactions**:

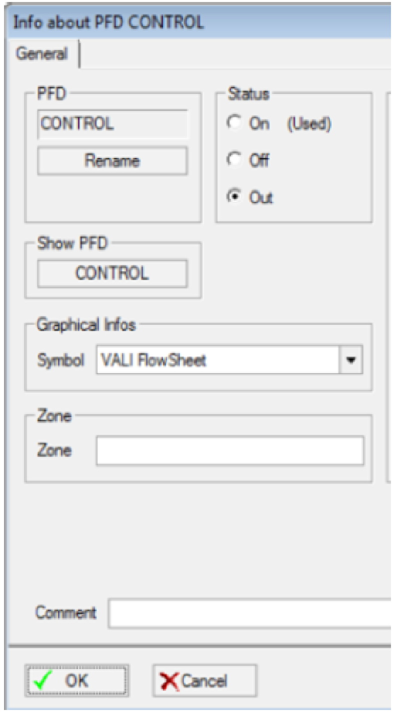
- Needed only when you use a reactor with a user defined reaction

EPFL

Vali modelling basics



Choose the **PFD/Unit status**..



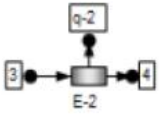
- **On:** the unit is operated normally
- **Off:** the UNIT does exist but is currently shutdown so that nothing flows to or from it. As a consequence, the streams connected to that unit will be shutdown as well
- **Out:** The UNIT is considered as not existing at all.
- **STREAMS** connected only to units that are OUT becomes OUT themselves, which means that they will not be part of the model during the next run

Commonly used Vali units

Heat Exchanger units: Require at least 1 material stream inlet, 1 material stream outlet and a thermal stream

SATVAL

- Used to obtain saturated fluid (i.e. saturated liquid or saturated vapor) in the outlet
- Outlet vapor fraction must be defined
- Possible to define superheating/subcooling



Name: HP_EVAP / HP   Category: Heat exchanger   Type: SATVAL

General | Parameters | Tags... | Reactions | Control Tags | Others | Flex code

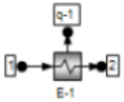
Parameters

Name	Description	Value	Physical Unit	Status
DPX	Nominal pressure drop	-1	bar	Input
MASSFX	Nominal mass flow rate	-1	kg/s	Input
CFDP	DP correction factor	1	-	Measurable
VFRAC	Vapour fraction (0,1)	1	-	Input
DT	Subcooling/Superhea...	0	K	Input

Default Values Parameters

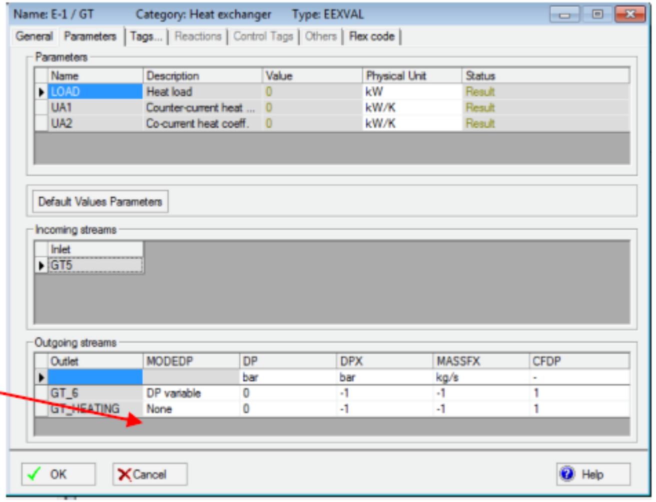
Commonly used Vali units

Heat Exchanger units: Require at least 1 material stream inlet, 1 material stream outlet and a thermal stream



EEXVAL

- A more flexible heat exchanger unit
- Compared to SATVAL more properties should be defined



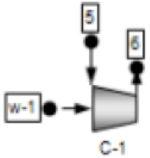
If Pin=Pout put DP variable to material outlet
Don‘t forget to specify DP=0 in the Tags tab

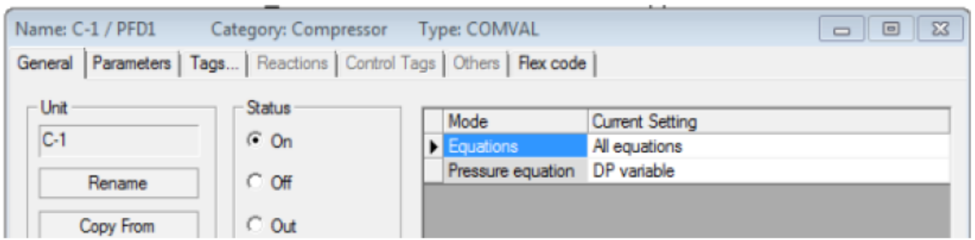
Commonly used Vali units

Compressors and valves

COMVAL

- Only compressor unit available on Vali
- Requires a material inlet, a material outlet and a mechanical stream
- Hint: don‘t forget to set Pressure equation DP variable





DPVAL

- Valve unit
- Requires a material inlet and a material outlet
- Hint: don‘t forget to set Pressure equation DP variable

Commonly used Vali units

Separation, blackbox units

LVEVAL

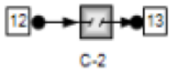
- Liquid-vapor separation unit on Vali
- Requires at least a material stream inlet and 2 material stream outles (1 liquid and 1 vapor)

BBXVAL

- Blackbox unit
- Very flexible: can be used with material streams, mechanical streams, thermal streams or combination of them

CUTVAL

- A type of Blackbox unit
- Used to break the material or pressure loops that can appear when dealing with closed cycles like for example the steam/water cycle in a power plant or a refrigeration cycle

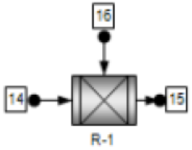


Commonly used Vali units

Reactor units: Require the reactants (e.g. air and natural gas) and products (e.g. fumes) as material streams

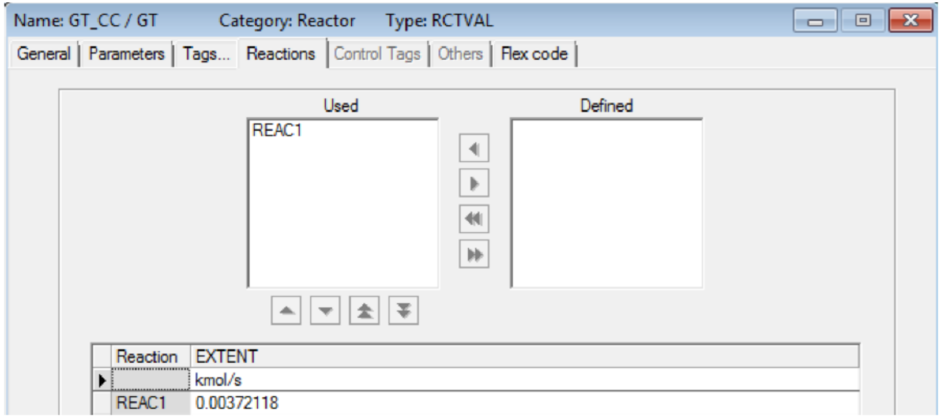
BATVAL

- A reactor unit that takes the atomic balances, energy balance and pressure drop into account
- Well suited for reactors with unknown reaction stoichiometry



RCTVAL

- Similar to BATVAL: takes the atomic balances, energy balance and pressure drop into account
- Used with user defined reactions



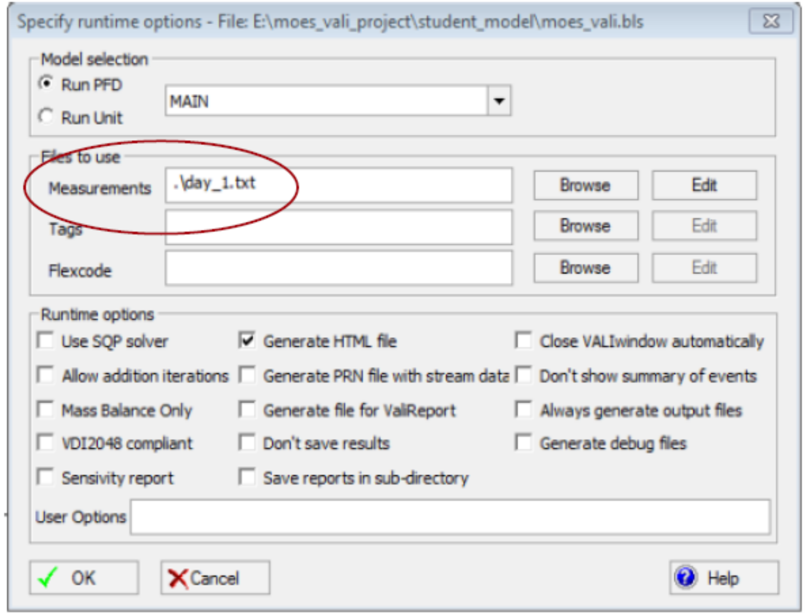
How to run a Vali model

Choose what you want to run (i.e. a PFD, a unit or the whole model)

Choose the measurement file that you want to run your model with (not obligatory)

Choose the run options:

- Generate HTML file is highly recommended as it creates a page with the errors in your model



EPFL

Vali input file – Measurements

DH_HEATING_LOAD	HP6_T	GT1_T	HP_ELECTRIC_VAR1	GT_ELECTRIC_VAR1	GT3_MASSF	HP1_MASSF	…
6438.6384	41.57307692	4.6	1670.83281	144.76501	0.017589718	29.435358	…
6212.7135	40.90384615	5	1656.75371	63.915238	0.008604093	28.534607	…
5647.9338	39.23076923	6	1392.58381	1.00E-05	1.00E-05	28.13084	…
3897.0433	34.04423077	9.1	898.07281	1.00E-05	1.00E-05	18.54226	…
0	22.5	16.1	1.00E-05	1.00E-05	1.00E-05	1.00E-05	…
0	22.5	18.6	1.00E-05	1.00E-05	1.00E-05	1.00E-05	…
0	22.5	20.1	1.00E-05	1.00E-05	1.00E-05	1.00E-05	…
0	22.5	19.6	1.00E-05	1.00E-05	1.00E-05	1.00E-05	…
903.66779	25.17692308	14.4	154.48681	1.00E-05	1.00E-05	4.3892858	…
2541.5621	30.02884615	11.5	516.42961	1.00E-05	1.00E-05	12.423414	
5309.058	38.22692308	6.6	1274.28001	1.00E-05	1.00E-05	25.653934	
7850.6021	45.75576923	2.1	1880.26801	606.75306	0.075659966	28.844983	

- EPFL heat demand data
- Heat pump refrigerant temperature at point 6 (HP6_T: see the figure in the project description)
- Air inlet temperature to the fuel cell (FC1_T)
- Net electricity consumption of the heat pump (HP_ELECTRIC_VAR1)
- Net electricity production of the fuel cell (GT_ELECTRIC_VAR1)
- Mass flow rate of the natural gas inlet to the fuel cell (GT3_MASSF)
- Mass flow rate of the heat pump refrigerant at point 1 (HP1_MASSF)
- Compression ratio of the first stage of the heat pump (HP_COMP1_PRATIO)
- Compression ratio of the second stage of the heat pump (HP1_COMP2_PRATIO)
- Mass flow rate of the heat pump at point 4 (HP4_MASSF)
- Mass flow rate of the fuel cell at point 1 (GT1_MASSF)

Vali input file – Measurements

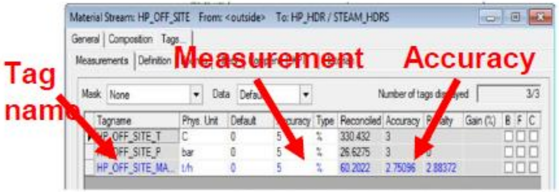
Giulia Giacomini

- Tag name: Specific name you used on your Vali model

- Measurement: measured value of the tag

- Accuracy: Measurement inaccuracy
  - CST: For the measurements that you want to keep constant
  - OFF: For the properties that you want Vali to calculate
  - - x: For the measurements with x% accuracy
  - x: For the measurements with x absolute accuracy

- Unit: unit of the measurement




```
HP_OFF_SITE_T     330.432114   -3.000000    C
HP_OFF_SITE_P     25.627524    -3.000000    barg
HP_OFF_SITE_MASSF     55.490597    -5.000000    t/h
HP_TO_VAL_MASSF 29.264033   -5.000000    t/h
HP_TO_HEX2_MASSF      5.248323     -5.000000    t/h
HP_TO_HEX3_MASSF      28.640145    -5.000000    t/h
LP_FROM_FT_P      4.106629     -3.000000    barg
LP_OFF_SITE_T     147.000000   -3.000000    C
LP_OFF_SITE_P     4.106629     -5.000000    barg
LP_OFF_SITE_MASSF     18.097119    -5.000000    t/h
LP_TO_HEX4_MASSF      17.248636    -5.000000    t/h
LP_TO_HEX5_MASSF      2.901057     -5.000000    t/h
LP_TO_HEX6_MASSF      0.412501     -5.000000    t/h
LP_TO_HEX7_MASSF      0.012194     -5.000000    t/h
MP_TO_HEX1_P      5.886748     -3.000000    barg
COND_FROM_FT_P    4.106629     -3.000000    barg
CUTOFF MASSF    0.015     t/h
CUTOFF VOLF    0.015     m3/h
ARCHIVE RUNS/365_RESULTS.TXT
DATA TAG
PENALTY
CHISQU
ARCHIVE VALI_OUTPUT_TAGS.TXT
DATA TAG
! Results Extracted at: 2015.11.5 18-47
```

Unit

Optional commands

To archive the results in a txt file

Info on the output file have to be included in the Vali input txt file. In the example, the generated output is called "365_results" and it will be stored in folder "runs". "DATA TAG" is a command that simply tells Vali to copy all the tags of the input files.