A new approach to process design *-- software --*

Heinz A Preisig

Process Systems Engineering @ Chemical Engineering

NTNU

NTNU, Trondheim, Norway

Process design -- roots

- Traditionally design views the plant as a combination of unit operations
- Design was focusing on continuous plants
- Unit operations -- a standard set of units
  - in functionality
  - in mechanical design

Process design == flowsheeting

Process → organised set of interacting units

- firstly mainly in a sequential pattern
- later more integrated
  - leading to lots of loops
  - leading to conversion problems
- two main solving approaches
  - sequential modular with recycle as latent streams
  - equation based
  - grey zone in between as equation based can be done in different ways also approaching sequential modular

Design & control

Lot’s of effort but principally in vain.

Why ?

Because of the intrinsic time separation.

- process is designed to operate in steady state
- control is to move each unit or group of units **fast** to the desired state == steady state

Dynamic control is limited to move the unit safely and quickly in a short time scale

Steering/planning is on a larger time scale and can be solved on yet a longer time scale assuming the plant is fast.

Side effects

- Limited technology for handling dynamic processes such as batch and semi batch
  ⇒ lack of discrete-event dynamic control
    - recipe implementation and control

- Applies also to continuous plants
    - startup
    - shutdown
    - exception handling → fault detection, isolation and counteraction / recovery or shutdown action

- Systematic methods for hazop analysis

Structural consequences

- Unit operations as base components
  ⇒ the behaviour is captured in a software module that solves the input/output operation of each unit

- Education's conservatism
  ⇒ mathematical models are emphasising the intensive properties (concentration and temperature, pressure)
  ⇒ transformed version of the conservation and balances are coded

- Economics of support
  ⇒ integration of modelling tools with numerical solvers in a closed package
  ⇒ a very few commonly used tools -- Aspen, HYSYS, ProSim, …

https://en.wikipedia.org/wiki/List_of_chemical_process_simulators

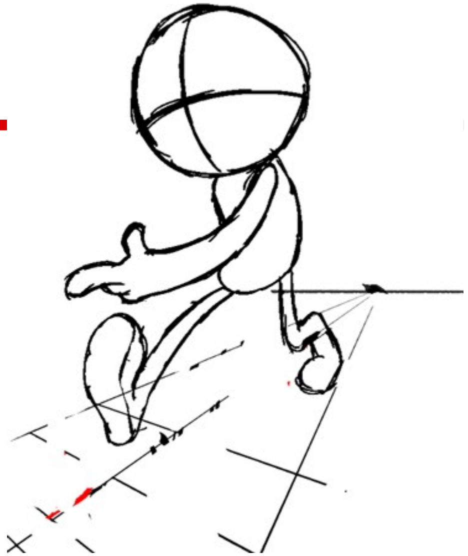
Design of bio processes

- Often dynamic processes (batch, fed batch) ⇒ dynamic simulator
- Untraditional units ⇒ make your own unit
- Extremely complex models for the bio-chemistry
  ⇒ surrogates & model reduction/simplification
  ⇒ nearly impossible to capture the behaviour in its entirety
      ⇒ crude models only
- Many and different materials
  ⇒ extremely costly to determine properties of mixtures
- Concentrated and weird and very diluted
  ⇒ both extremes quite common
- Not much of an idea on what combination of operations, bio-chemistry, products yields a “good” process

Needs

- High flexibility
- Fast construction of unit operation models
- Fast construction of plants
- Inheritance of models
- Different target environments
- Minimization / elimination of errors
  - in model basics behaviour description
  - model structure
  - code generation
  - no “silly” problems like underdetermined of overdetermined or index problems

Approach



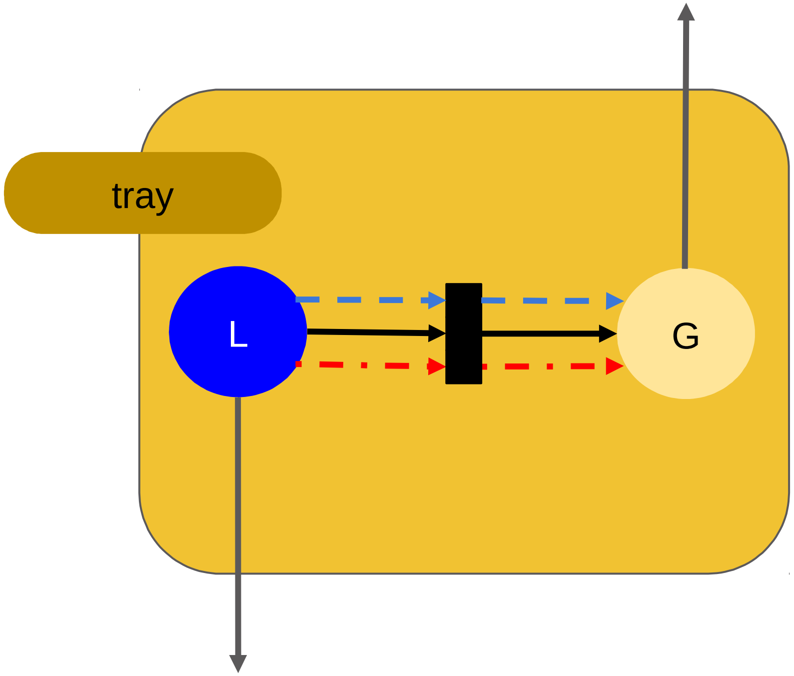
Walk backwards towards the roots of the behaviour description

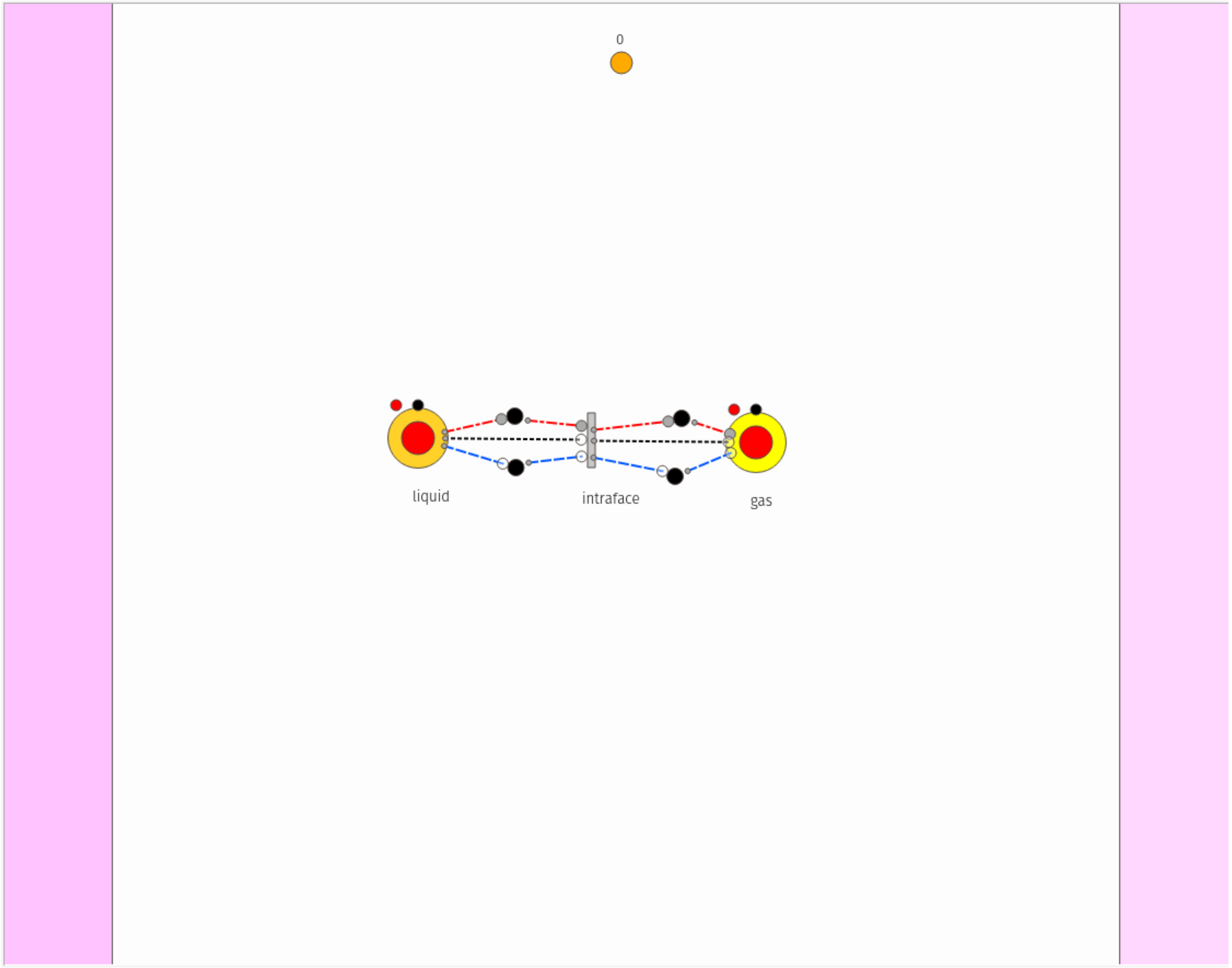
⇒ conservation principles
applied to principle control volumes

Constructing a unit operation model

Example: Distillation column

construct a tray




0
liquid
intraface
gas

Next level in the hierarchy

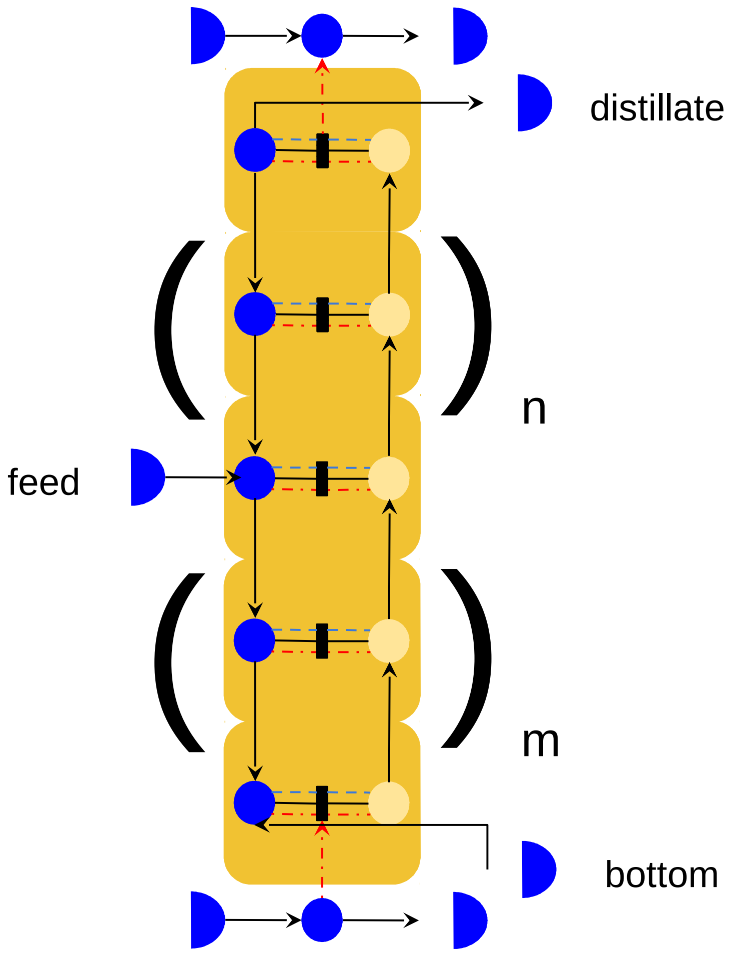
Stacking up the stages

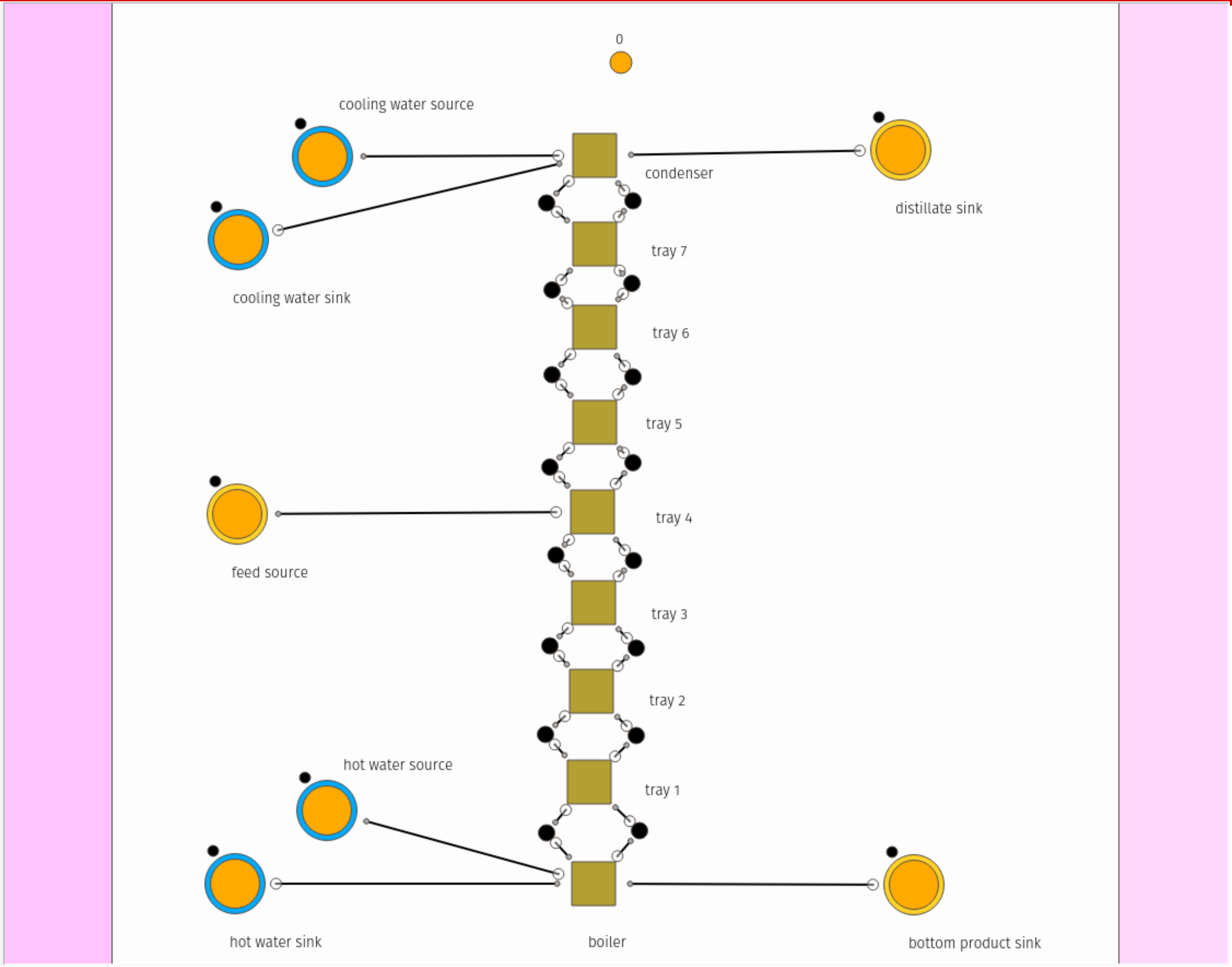
and

adding

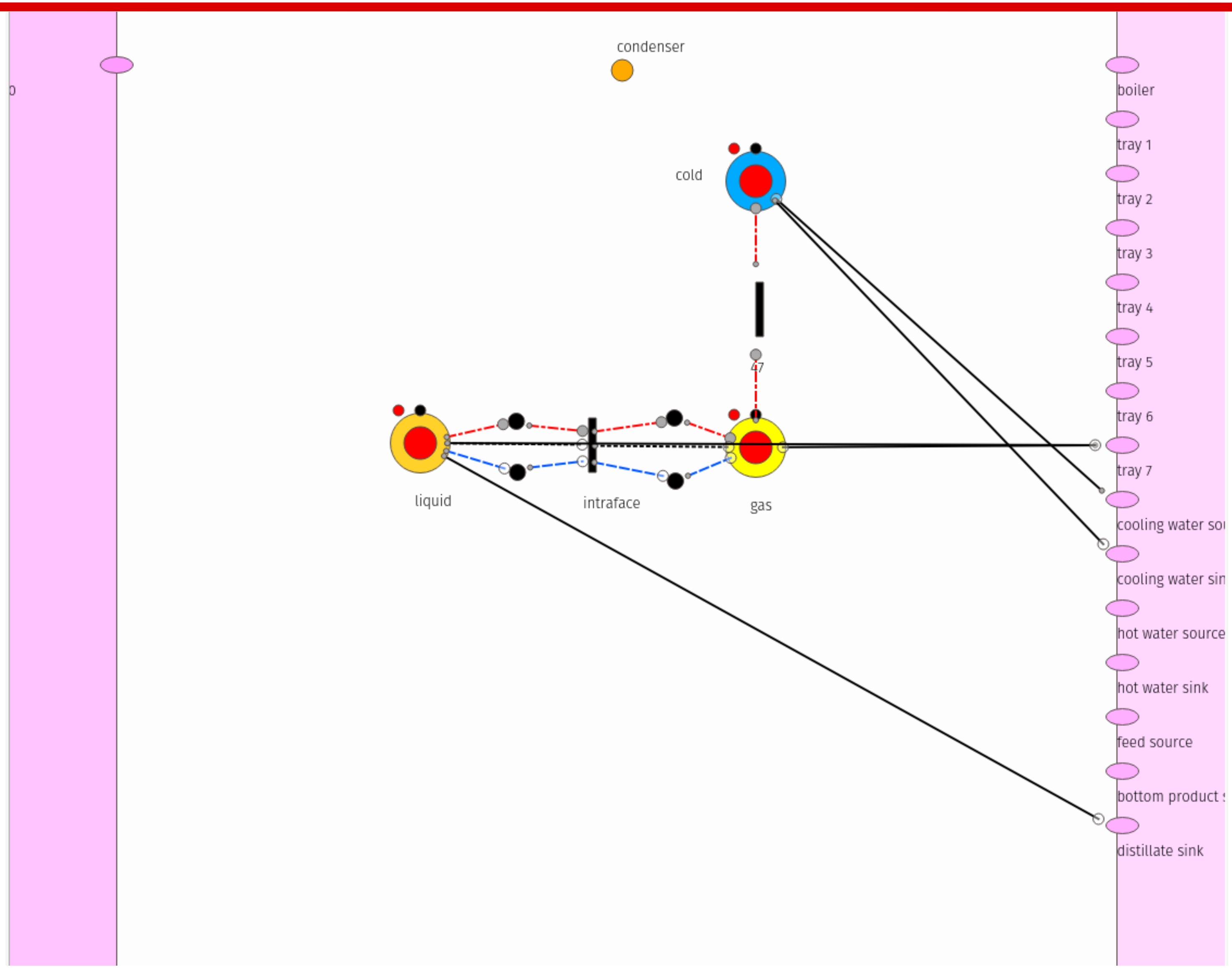
- boiler
- condenser
- feed stream
- distillate stream
- bottom product stream

completes the distillation model



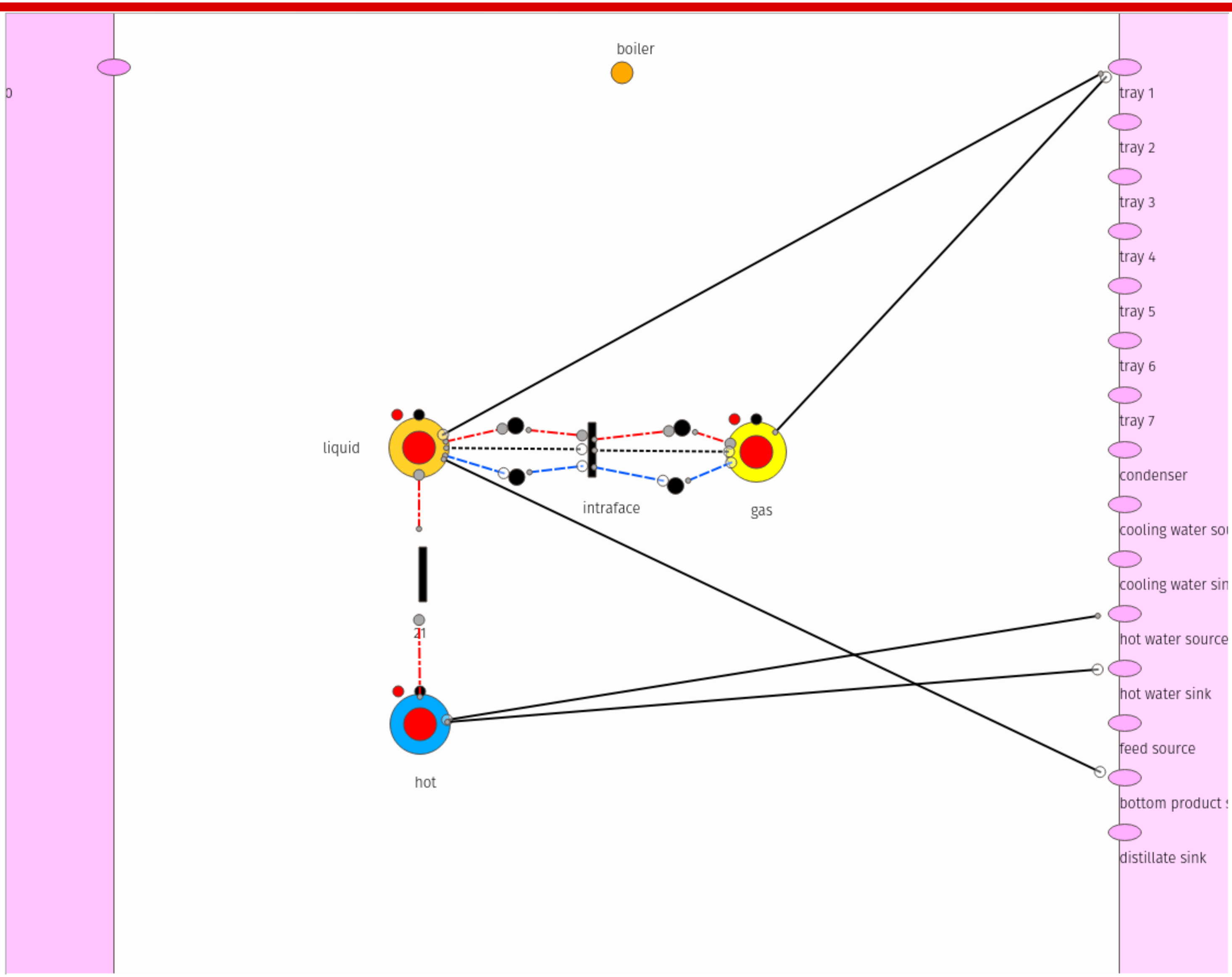

0
cooling water source
condenser
distillate sink
cooling water sink
tray 7
tray 6
tray 5
tray 4
feed source
tray 3
tray 2
hot water source
tray 1
hot water sink
boiler
bottom product sink

Condenser



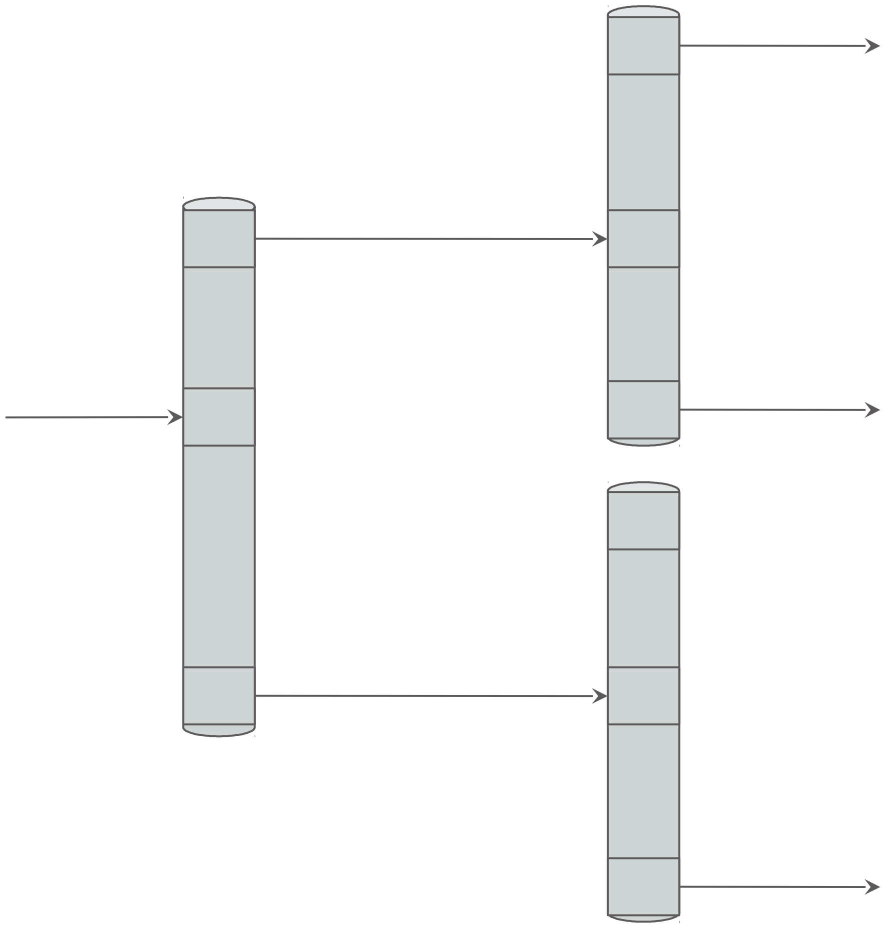
condenser
boiler
tray 1
tray 2
tray 3
tray 4
tray 5
tray 6
tray 7
cooling water so
cooling water sin
hot water source
hot water sink
feed source
bottom product
distillate sink
cold
47
liquid
intraface
gas

Boiler

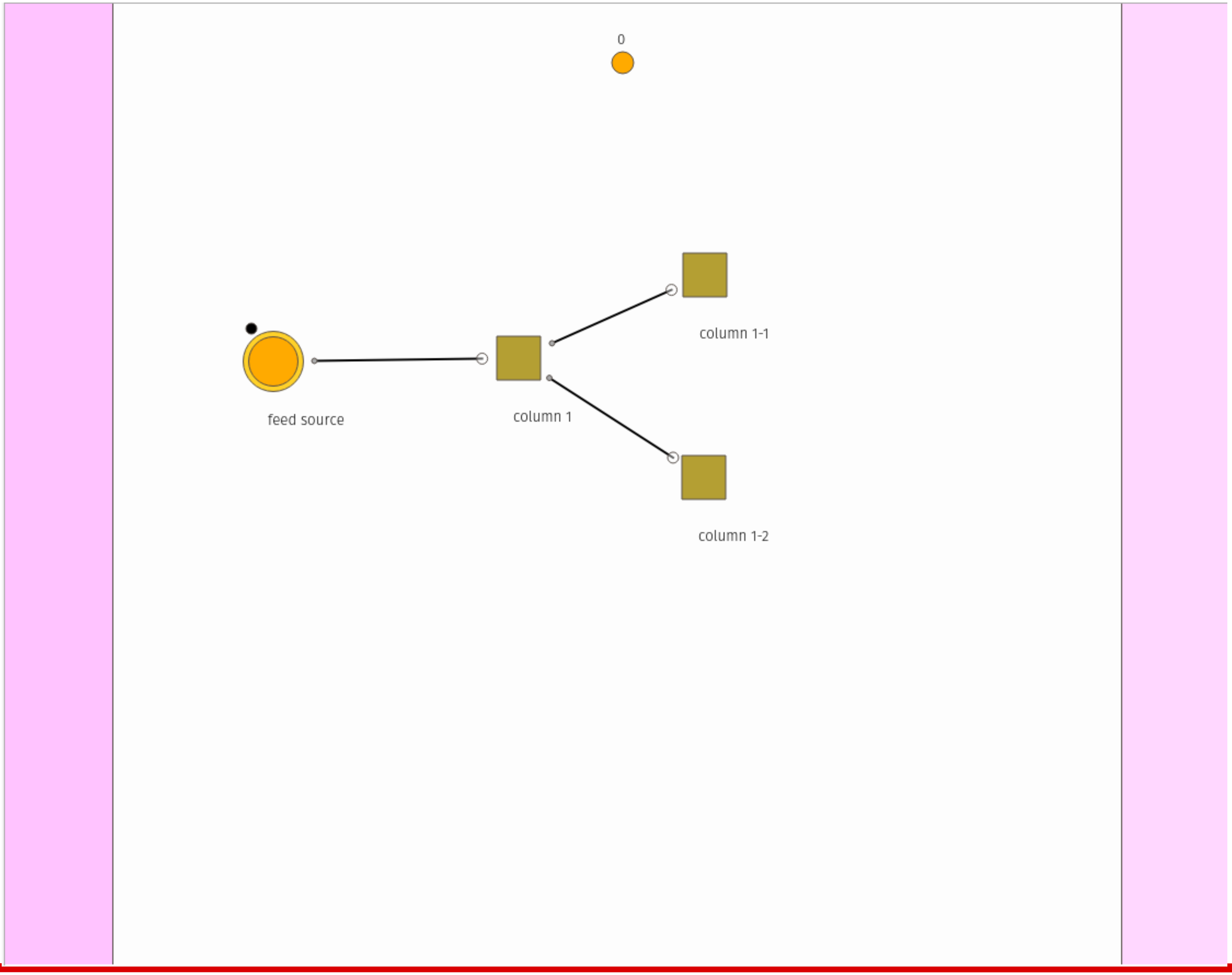


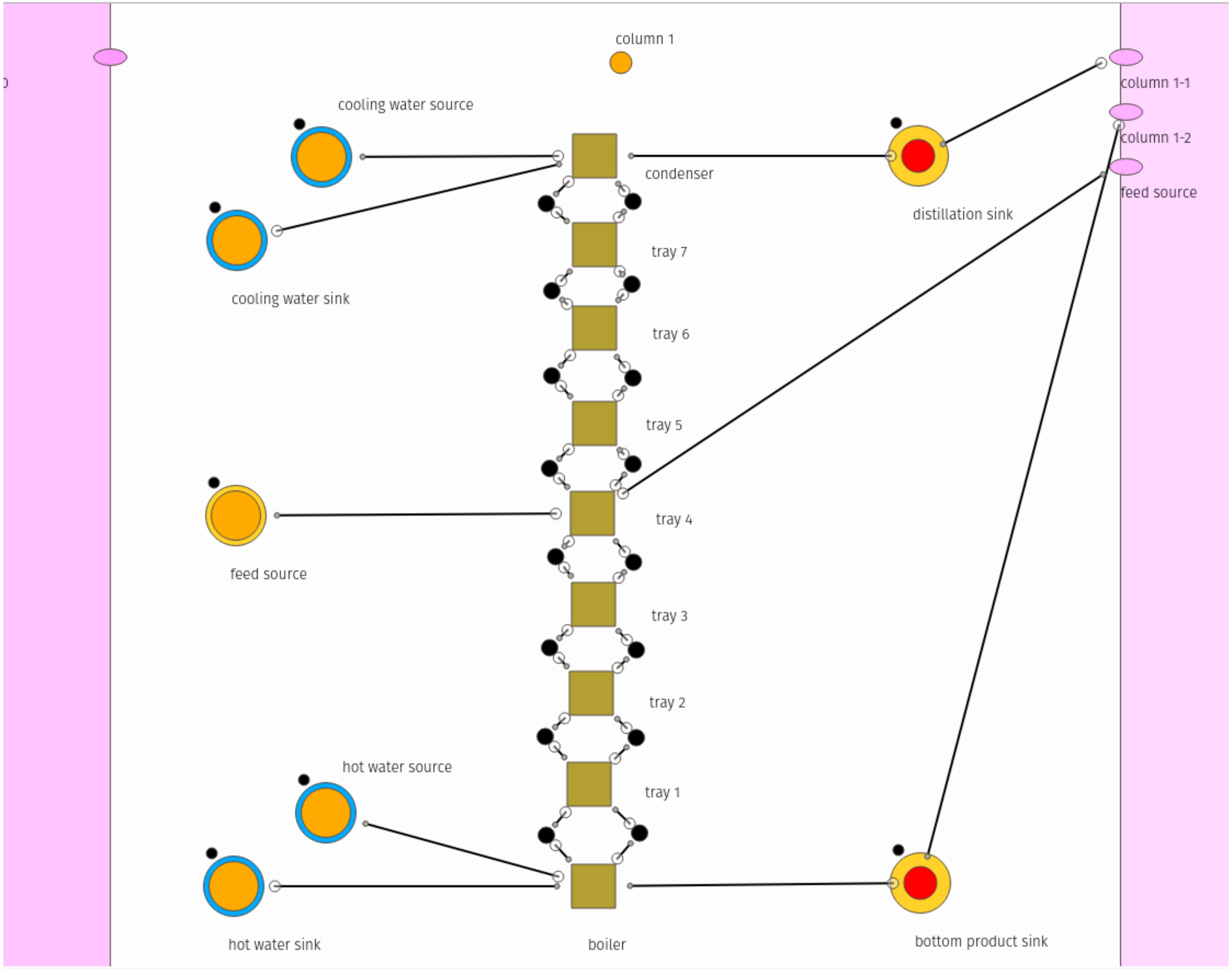
boiler
liquid
intraface
gas
hot
21
tray 1
tray 2
tray 3
tray 4
tray 5
tray 6
tray 7
condenser
cooling water so
cooling water sin
hot water source
hot water sink
feed source
bottom product
distillate sink

Next level -- a distillation train



Distillation train




column 1
cooling water source
condenser
distillation sink
column 1-1
column 1-2
feed source
cooling water sink
tray 7
tray 6
tray 5
tray 4
feed source
tray 3
tray 2
hot water source
tray 1
hot water sink
boiler
bottom product sink

Distillation -- summary

- Recursive construction
  - from tray ⇒ column
  - from column ⇒ to train

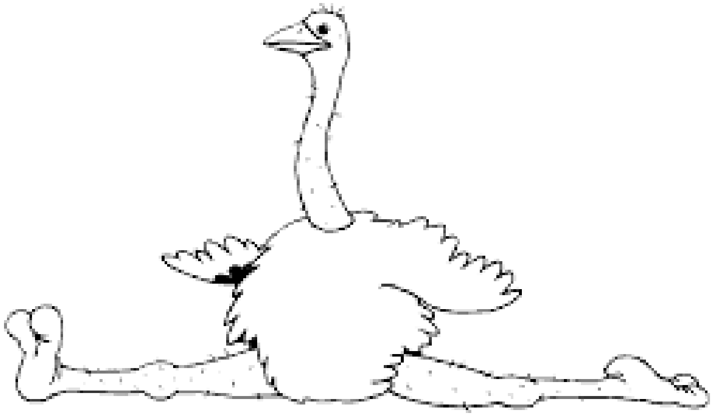
- Column at this stage is “empty” and can be populated with any mixture
- Adding species is done with a colouring algorithm spreading the species in the topology
- Corresponding component mass balances are coupled til
- Code is generated automatically
- Simulation after instantiation of parameters have been done

Further possibilities:

- Distillation with species can be saved and used in other models
- Instantiated model ditto

Spagat over scales and disciplines

Design must expand its domain:



- increasingly more material properties from molecular dynamics
- use different computational tools to solve multi-scale or multi-physics problem by generating a workflow for a matching platform
  ⇒ MarketPlace Horizon2020 EC project (2018-2022)
- Integration with optimisation
- Extension to control design (literature -- thermodynamic-based design and port-Hamiltonian systems)
- wider interaction, for example from CFD to 3-D printing

What’s so different ?

Standard approach:

- unit behaviours are defined
  dynamic ⇒ differential algebraic equation sets (DAE)
  static ⇒ algebraic equation sets (AE)

- flowsheet is assembled yielding flow matrix and units being used

- equation set for the simulated plant is
  - collected
  - analysed for index problems
  - analysed for degree of freedom
  - ordered
  - ⇒ submitted to numerical solver

It is different

Our approach:

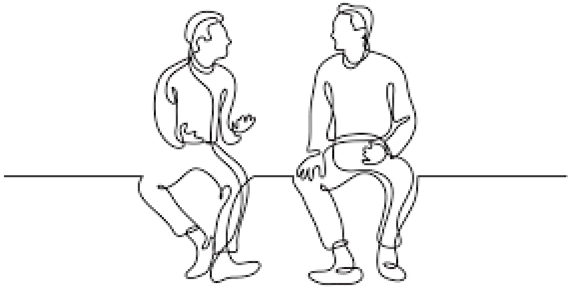
- ontology defines domain structure
  ⇒ physical → phases & material
  ⇒ control → continuous, sampled-data, event-driven
- ontology is augmented with equations forming a lower triangular equation system
  ⇒ keeps it proper in terms of units and indexing
  ⇒ defines the computational sequence
  ⇒ compilation is done at this stage
- plant model is assembled graphically
  ⇒ produces index sets only
- solver gets
  - compiled and indexed equation set from ontologies
  - instantiation information (initial conditions, parameters etc)

Advantages for the user

- Use of ontology ⇒ guaranteed **proper** model
  - degree of freedom = 0
  - no index problems
  - closure of the conservation guaranteed at convergence
  - no compilation errors
  - ontology disables structural errors within user-defined topology
  - topology construction is constraint by topology to disable structural errors
- Extremely flexible library function
  - just topology
  - topology with species
  - coupling to material models
  - coupling to control structures
- Proper integration of control and material models
- Scale separation and link to other scales enabled

Side effects -- splitting the work

- Work is split into two distinct domains
  - constructing the ontology
  - modelling plants



Constructing the ontology requires the input from the specialist

- macroscopic physical chemistry
- molecular physical chemistry
- thermodynamics
- fluid mechanics
- separation technology
- reactor technology
- control technology
- ecology

Constructing plants

- plant insight
- chemistry and biology
- generating alternatives
- analysis of the results

- enabled to work with different disciplines
- fast and effective in generating alternative solutions

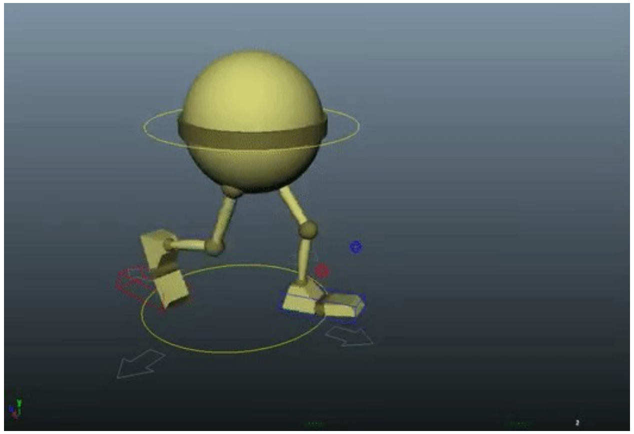
Technical side effects

Different business model

- ontology generation split from model generation split from solver technology

- model structure in terms of what equation is used where carries all the way through
  - enabling using different solver technologies for different parts
  - enabling a more detailed analysis of the results

- enables distributed computing
  - molecular modelling on one
  - fluid dynamic on another one….



Do we need it for bio processes?

exotic units ?

⇒ constructing your own units is supported not inhibited

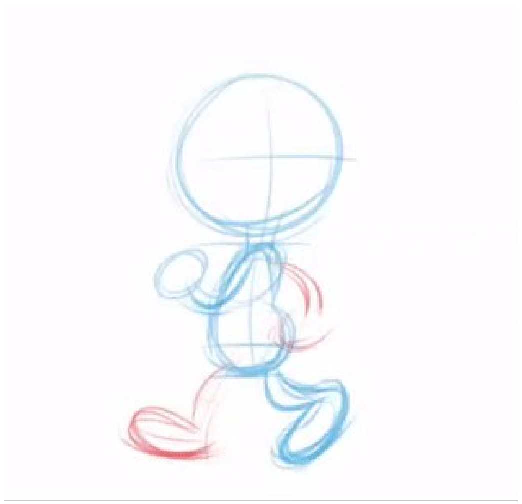
quick on generating alternatives ?

⇒ models on different levels:

sections, units, ..

with or without species included

instantiated or not …



strange mixture properties ?

⇒ open for including any type of material models

from simplistic to any level of sophistication

design and control ?

⇒ fully integrated

Something to think about
Thank you for attending

Thank you for attending