American Modelica Conference 2022

MATERIAL PRODUCTION PROCESS MODELING WITH AUTOMATED MODELICA MODELS FROM IBM RATIONAL RHAPSODY

Dr. John Batteh, Jesse Gohl, James Ferri, Quang Le, Bill Glandorf, Bob Sherman, and Rudolfs Opmanis

Modelon

VCU

P&G

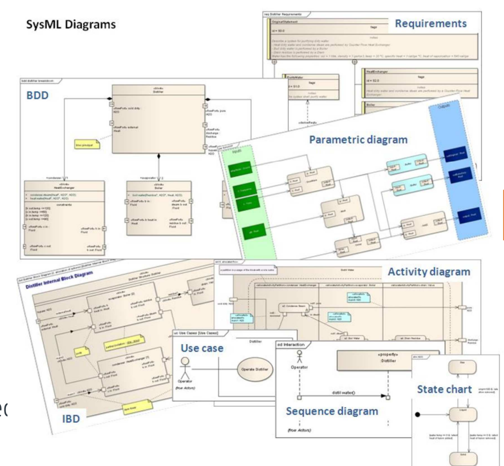
Tom Sawyer Software

AGENDA

- Motivation
- Modeling overview
- Modeling work
  - Component overview
  - System models
- Sample use case
- Conclusions

MOTIVATION

- Increasing complexity of modern manufacturing systems has led to paradigm shift from document-centric systems engineering to Model Based Systems Engineering (MBSE)
- Multidisciplinary Design Analysis and Optimization (MDAO) focuses on creating an analysis model to demonstrate system behavior via dynamic simulations
- Gap between approaches
- Goal: author dynamic simulation model from structural model
    - Develop infrastructure to automatically generate simulations via Modelica models from manufacturing architectural model in SysML

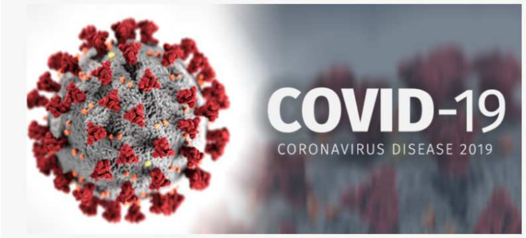


Modelica
Language

Modelon

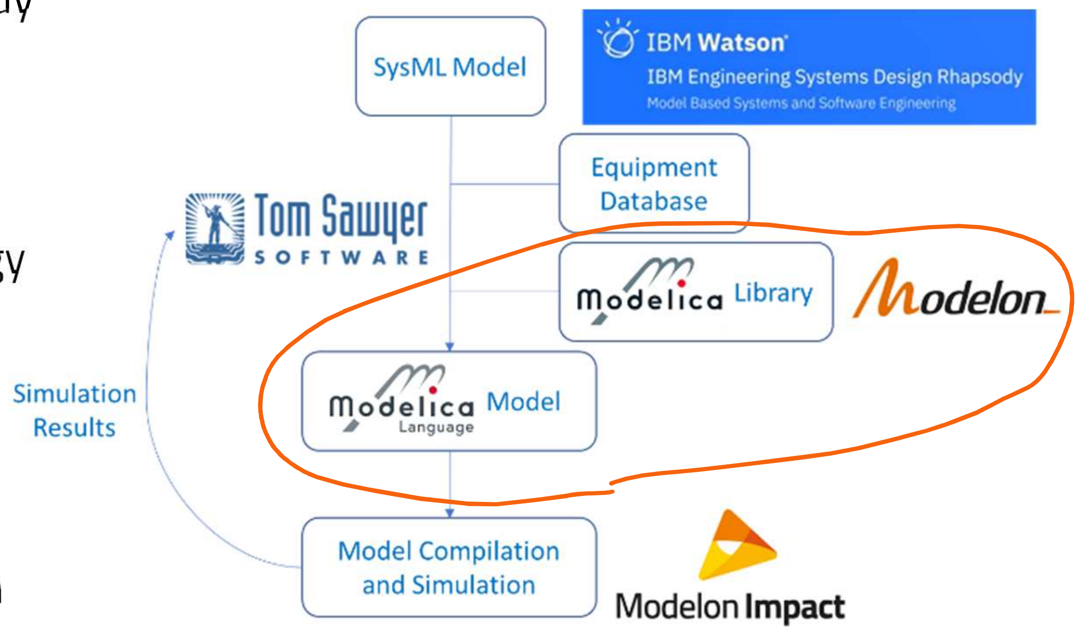
PROJECT

- U.S. Defense Advanced Research Projects Agency (DARPA) project to build digital infrastructure for improved efficiency in chemicals and materials industry
  - Make it easier for chemical manufacturers in the U.S. to produce critically needed medicines
  - Allow manufacturers to explore production duration, synchronization, requirements, and constraints to improve and optimize chemical synthesis processes
  - Address challenges in chemical industry to encourage domestic production of medications and broad range of active pharmaceutical ingredients (APIs) for drugs in U.S., instead of overseas
  - Drugs include in-demand APIs related to COVID-19 and several others on federal government's Strategic National Stockpile list



MODELING OVERVIEW

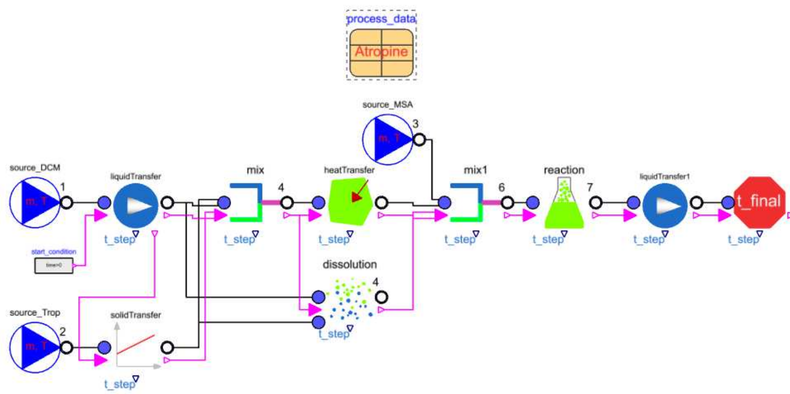
- SysML model created in IBM Rational Rhapsody that outlines manufacturing process steps
- Based on SysML model and equipment database for chemical plants, fully parameterized Modelica model automatically created using Tom Sawyer Software technology based on Modelica model library for various process primitives
- Resulting Modelica model simulated in Modelon Impact using its simulator API
- Key simulation results, including process throughput and process time, returned to Tom Sawyer Software for visualization and optimization regarding manufacturing process and equipment allocation



Modelon

MODELING APPROACH

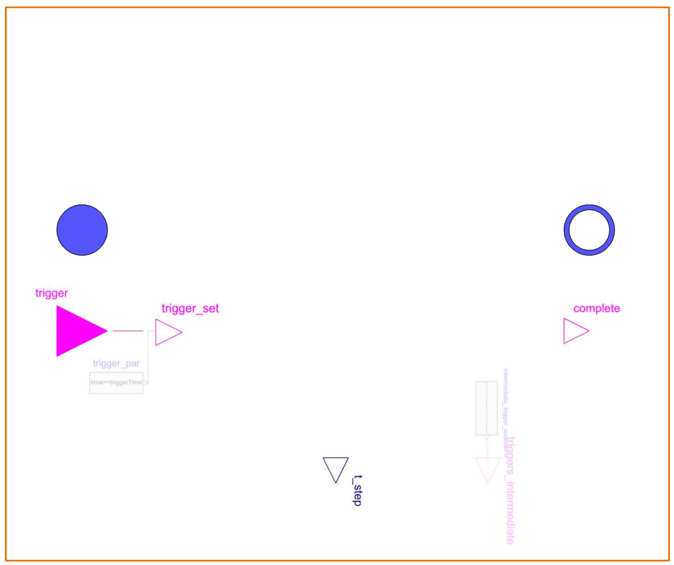
- Models focused on manufacturing process layout for analyzing process time and yield for batch-based material processes
- Challenges
  - Process steps for manufacturing pharmaceutical ingredients not wholly documented in public references
  - Models expected to be used in massive optimization processes
- Models intentionally implemented to be computationally fast due to low fidelity implementations and use of time events



PROCESS STEPS

- Represented as individual primitive components
- Each stage computes its status (complete) and material characteristics based on stage physics
- Material characteristics and status feed successive stages
- Stages are ordered -> causal interfaces

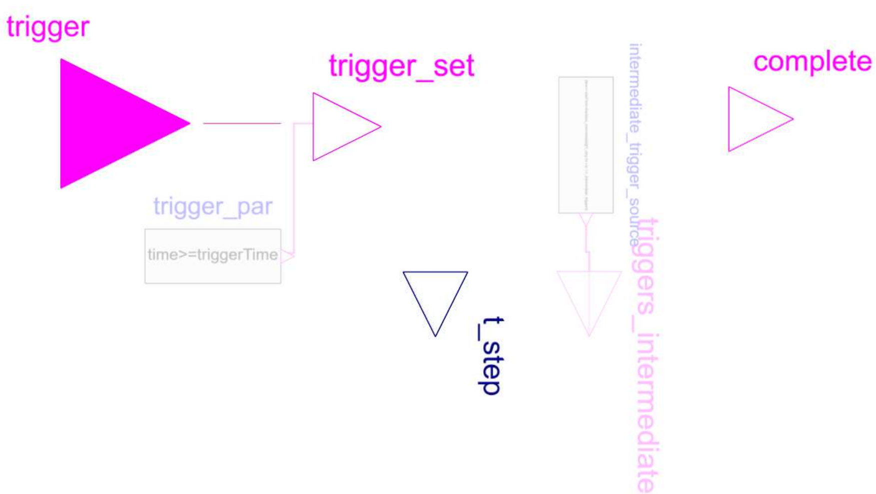
```
connector ProcessInput "Process stage input material characteristics"
  input Integer species_index "Material species identifier index";
  input Modelica.Units.SI.Mass mass "Material mass";
  input Modelica.Units.SI.Temperature T "Material temperature";

  annotation (•••);
end ProcessInput;
```




```
connector ProcessOutput "Process stage output material characteristics"
  output Integer species_index "Material species identifier index";
  output Modelica.Units.SI.Mass mass "Material mass";
  output Modelica.Units.SI.Temperature T "Material temperature";
  annotation (•••);
end ProcessOutput;
```

LOGICAL INTERFACE

- Stages share status with adjacent steps via `complete` variable
- Stage can depend on multiple previous steps so input `trigger` is Boolean array
- Processing begins when all triggers are true, process internal timer started
- Conditional option for time-based triggers via parameter



MATERIAL DATA RECORD

- Simplified approach for material representation due to lack of rigorous species information and property data in development of API
  - Species array
  - Thermophysical properties
- Used as inner/outer

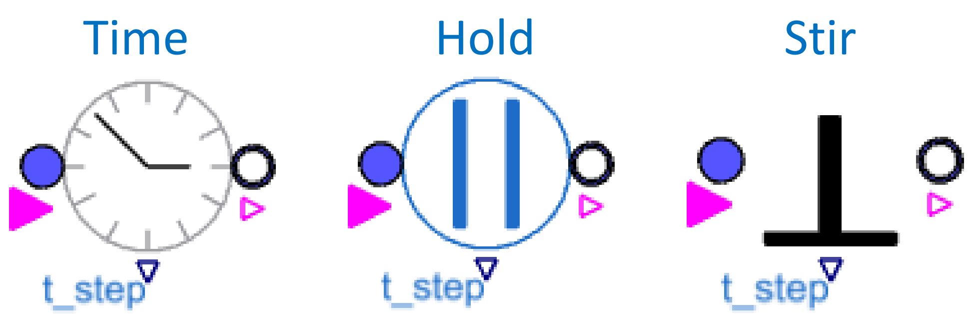
```
record Base
  extends Modelica.Icons.Record;
  final parameter Integer ns=size(species_names,1) "number of species";
  parameter String species_names[:] "species names";
  parameter Modelica.SIunits.MolarMass MW[ns] "Molecular weights (kg/mol)";
  parameter Modelica.SIunits.Density rho[ns] "density";
  parameter Modelica.SIunits.ThermalConductivity lambda[ns] "thermal conductivity";
  parameter Modelica.SIunits.DynamicViscosity mu[ns] "absolute viscosity";
  parameter Modelica.SIunits.SpecificHeatCapacity cp[ns] "specific heat";
  parameter Modelica.SIunits.DiffusionCoefficient D[ns] "diffusion coefficient";
  parameter Modelica.SIunits.SpecificEnthalpy Hv[ns] "latent heat of vaporization";
  parameter Modelica.SIunits.Temperature Tv[ns] "vaporization temperature at standard conditions";
  parameter ASKPSP.Types.MatterState state[ns] "state of matter";


  annotation (...);
end Base;
```

Index	Species
1	DCM
2	Tropine
3	Methanesulfonic acid
4	DCM+Tropine
5	DCM+Methanesulfonic acid
6	DCM+Tropine+Methanesulfonic acid
7	DCM+Tropine methanesulfonate

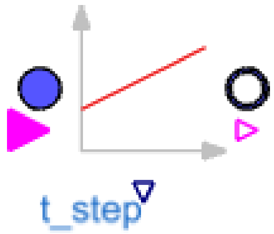
TIME COMPONENT

- Simple time-based with fixed time delay
- Pure delay with no material modifications
  - Same material species leaves that entered
  - No mass is stored in the component
  - No heat is transferred.
- When stage is complete, outlet mass and temperature become same as inlet

```
partial model TimeComponent "base class for a time based component"
  extends TriggeredComponent;
  parameter Modelica.Units.SI.Time tau "time for process";

equation
  t_step = tau;
  complete = time >= startTime + tau;
end TimeComponent;
```

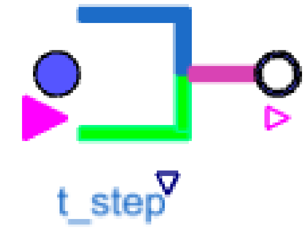


RATE COMPONENT



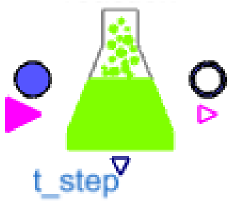
- Stages that operate at prescribed rate
- Processing time computed based on rate equation using ratio of the total quantity to be processed and processing rate
- Fixed rate specified via parameter

MIX COMPONENT



- Uses component array inputs
- Simulate stages where multiple materials are combined over fixed amount of time
  - New, outgoing species is specified by a parameter
  - Outgoing mass is conserved as the sum of incoming masses
  - Temperature of the outlet material mass-average of incoming materials (note: not a rigorous conservation of energy due to lack of detailed information about process species at each stage)

REACTION COMPONENT



- Combines multiple materials to produce a new outgoing species
- Parameters
  - Output species
  - Reaction time
  - Yield fraction
  - Reaction temperature change

VOLUMETRIC RATE AND LIQUID TRANSFER

- Volumetric Rate
  - Simulates fixed volumetric flow rate for incoming material
  - Density of incoming material used along with incoming mass to compute material volume to be transferred
- Liquid Transfer
  - Similar to Volumetric Rate
  - Volumetric flow rate calculated based on hydraulic flow through smooth pipe driven by constant power pump

$$Re = \frac{4\rho Q}{\pi \mu D}$$

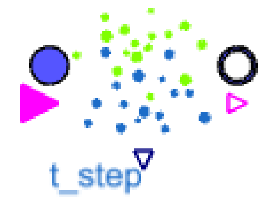
$$\Delta p = \frac{2\rho f L v^2}{D}$$

$$f = 0.0791 \cdot Re^{-1/4}$$

$$Q = v \cdot A$$

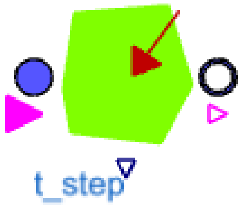
$$P_b = Q \cdot \Delta p$$

DISSOLUTION



- Computes duration required to fully dissolve specified mass of solute in stirred, fixed volume vat
- Solute can be specified either as a fixed parameter or entered from conditional connector
- Time for dissolution calculated based on mass transfer analysis for a stirred vessel

HEAT TRANSFER



- Assumes liquid in fixed volume, stirred vessel
- Calculates time required to bring material to new temperature given initial temperature and temperature of heat transfer fluid

$$\Delta H = Q = C_p \Delta T = C_p (T - T_0)$$

$$\dot{Q} = C_p \dot{T} = hA(T_{ht} - T)$$

$$T(t) = T_{ht} + (T_0 - T_{ht}) e^{-t \frac{hA}{C_p}}$$

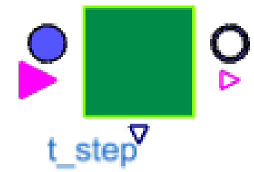
$$t_f = -\tau \log\left(\frac{T_{ht} - T_f}{T_{ht} - T_0}\right)$$

DRYING FIXED RATE

- Accounts for addition of heat to evaporate fraction of incoming stream and change of species for output stream
- Species change depends on whether evaporate or dessicate (remainder) continues to outlet or is discarded
- Handles both drying and distillation
- Assumes fixed rate heat transfer specified via parameter
- Process time accounts for duration to add sensible heat to raise temperature of both evaporate and dessicate and to add latent heat of evaporate

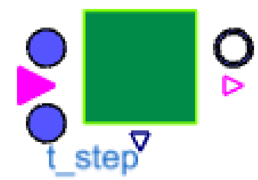
FILTER/WASH

- Filter
  - Uses Darcy's Law to model flow rate of solvent through permeable solid
  - Relates volumetric flow rate of a liquid to hydraulic permeability, cross sectional area, dynamic viscosity, flow length, and pressure difference

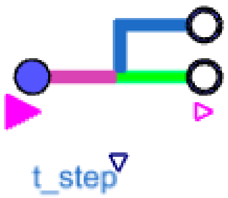


$$\Delta t = \frac{\Delta V \rho g}{A \Delta p} \cdot \left(\frac{L_f}{K_f} + \frac{L_c}{K_c} \right)$$

  - Outlet mass is solute mass computed from fixed yield fraction of filtration
- Wash
  - Extends from Filter but adds separate connection for solvent
  - Outlet temperature specified via parameter
  - Completion requires that all solvent must be delivered first



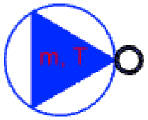
PHASE CUT



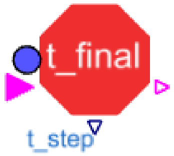
- Represents process separation step
- Splits material on input connector into two separate outputs based on prescribed fraction
- Yield fraction accounts for losses that occur in separation process

SOURCE AND END

- Source
  - Provides fixed amount of mass at a fixed temperature and specified species
  - No complete signal as it is material source
  - Delivery time accounted for by downstream transfer component

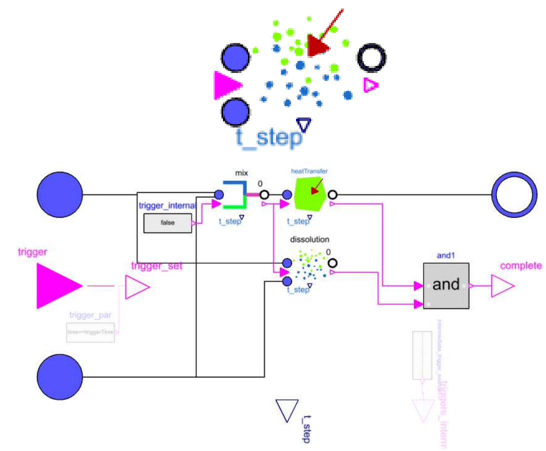


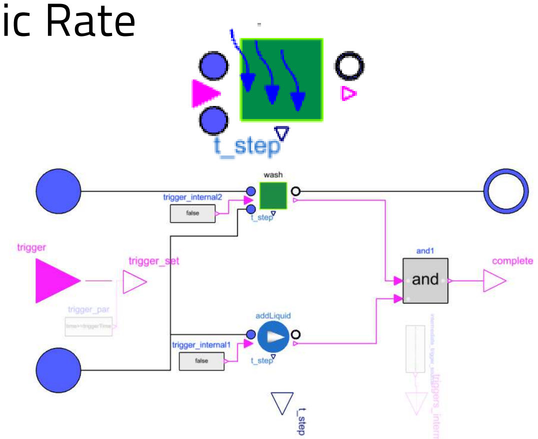
- End
  - Records overall completion time in discrete variable `t_final` when component is triggered
  - Terminates simulation
  - Final production species, mass, and temperature on input connector



COMPOSITE STAGES

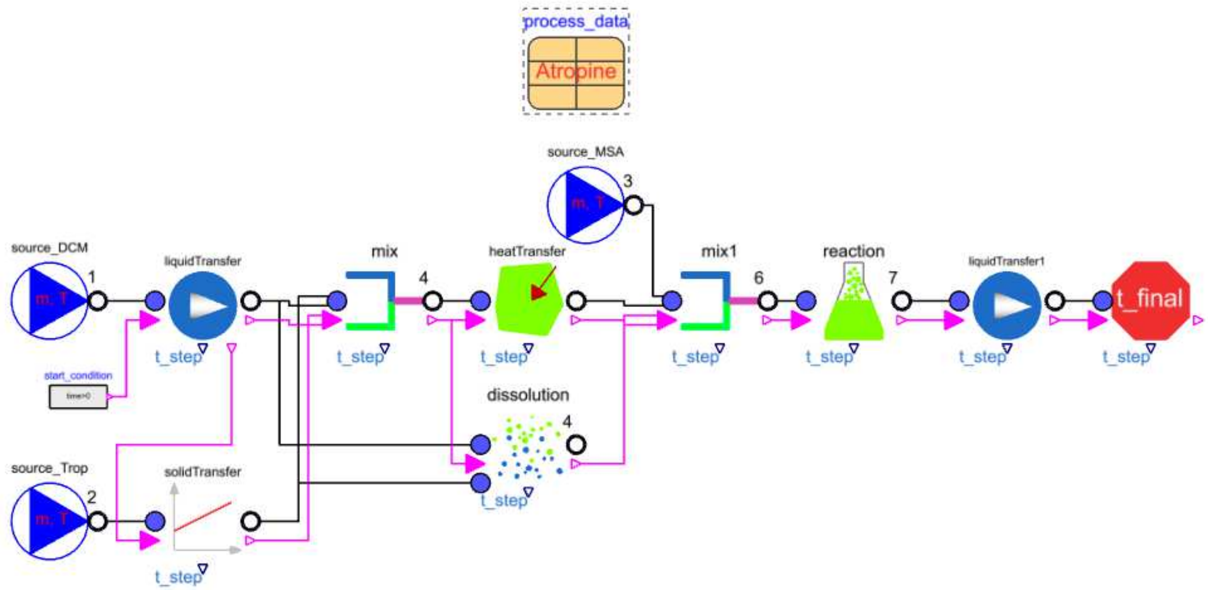
- Represents combinations of processes that are often performed together
- Reduces effort for automated code generation
- Heat Transfer and Dissolution
  - Dissolution processes often specify simultaneous heating
  - Dissolution isothermal so combined with heat transfer
- Add Liquid and Wash
  - Washing requires addition of liquid
  - Combines Wash with Volumetric Rate





PROCESS EXAMPLE

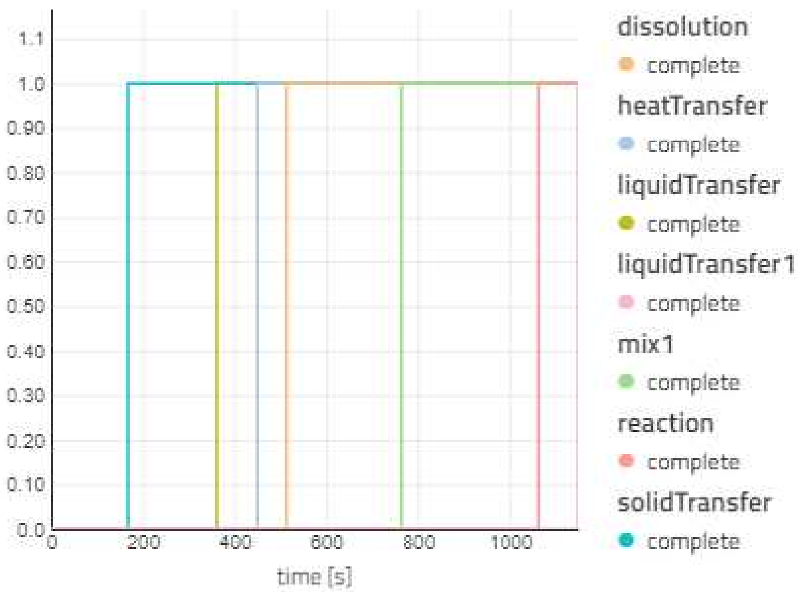
- Synthesis of tropine methanesulfonate, a precursor in synthesis of atropine
  - Add dichloromethane (DCM)
  - Add solid tropine
  - Mix
  - Heat mixture
  - Dissolve tropine in solution
  - Add methanesulfonic acid
  - Mix
  - Reaction
  - Transfer from reaction vessel

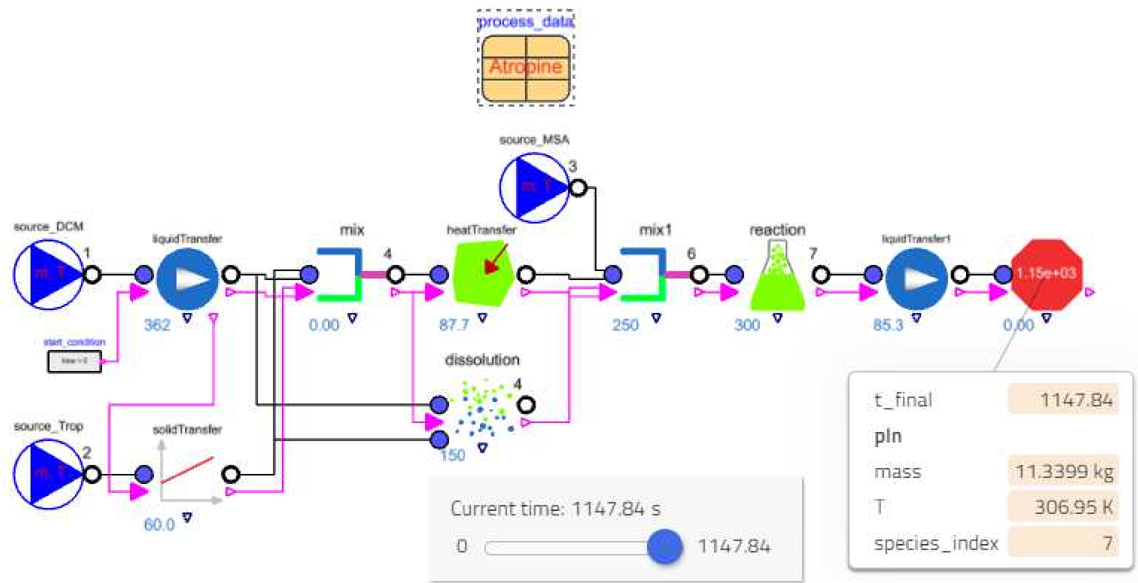


What is Atropine and how is it used?

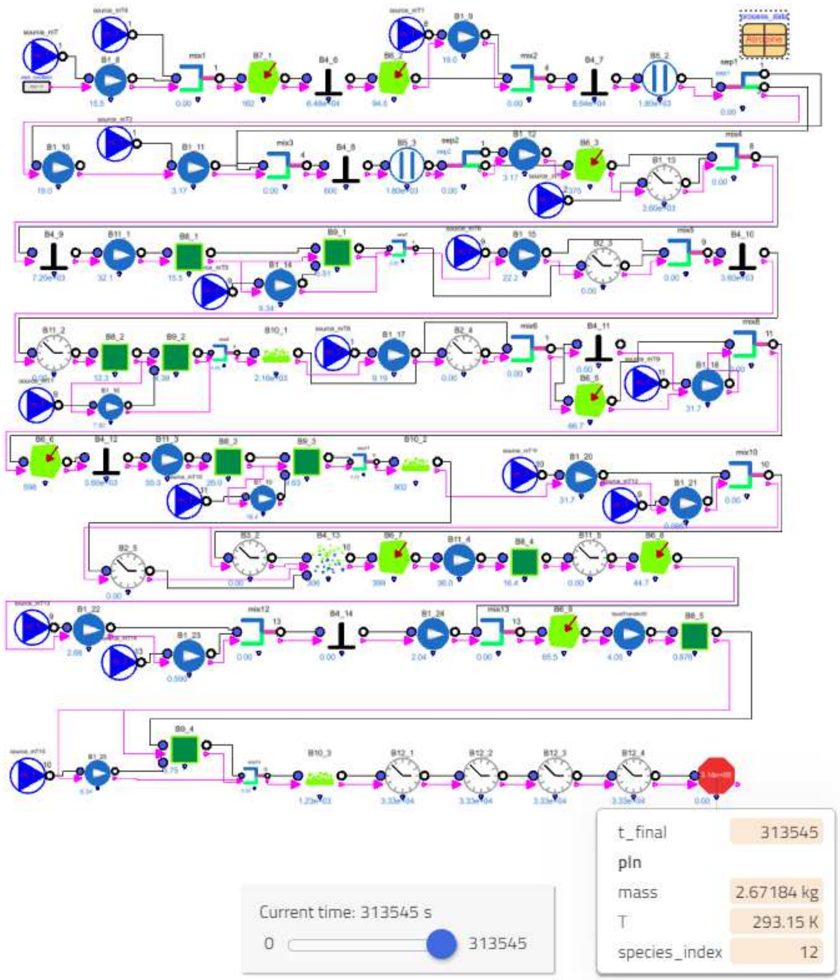
Atropine is a prescription medicine used to treat the symptoms of low heart rate (bradycardia), reduce salivation and bronchial secretions before surgery or as an antidote for overdose of cholinergic drugs or mushroom poisoning. Atropine may be used alone or with other medications.

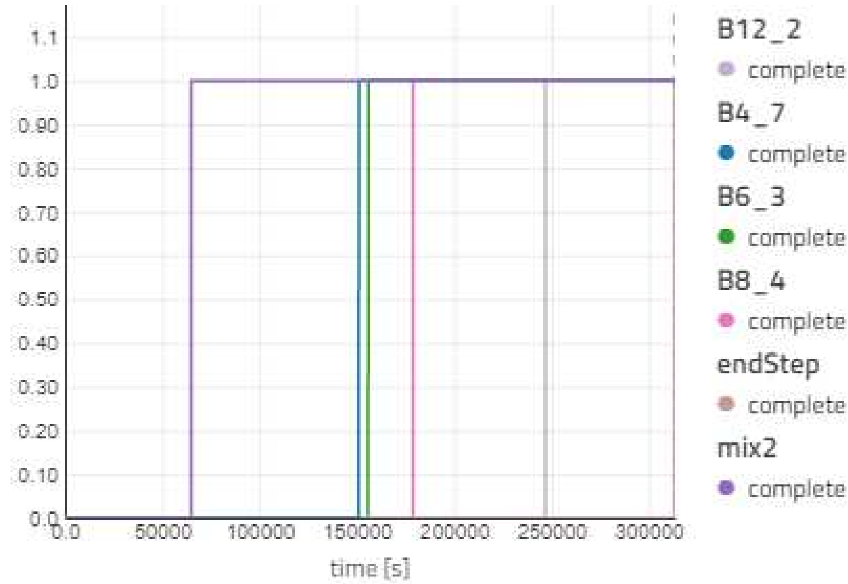
PROCESS EXAMPLE





ATROPINE SYNTHESIS





CONCLUSIONS

- Developed library to support DARPA project for digital infrastructure for chemical and materials industry
- Library integrated into software stack to automatically create process models from SysML models and simulate with Modelon Impact
- Demonstrated initial use case for atropine synthesis

- Future work to focus on analyzing supply chain, identifying capability gaps in key drug manufacturing, and optimizing production process
- Future publications to focus on SysML – Modelica capability


THANK YOU !