Quick Guide

What is this toolbox for:

Free-radical copolymerization toolbox can be used to simulate binary copolymerization reactions in semi-batch reactors under the following hypotheses:

- Isothermal, perfectly mixed reactor;
- Terminal kinetic model;
- No penultimate kinetic effects;
- Long chain approximation;
- Radical stationariety.

Content

This toolbox comes as a .zip file which contains the core files:

```
semi_batch_ODE.m
Mayo_Lewis_equation.m
conversion_target_event.m
CLD_and_MWD_reconstruction.m
logspacing.m
BinaryCopolymerizationSystem.m
Database.m
Database.mat
```

And the example files:

```
BATCH_OPERATION.m
BATCH_OPERATION_HOMOPOLYMERIZATION.m
BATCH_OPERATION_DEPROPAGATION_COMPARISON.m
SEMI_BATCH_OPERATION.m
CONTROLLED_SEMI_BATCH_OPERATION.m
SEMI_BATCH_OPERATION_FEED_TIME_COMPARISON.m
constant_feed_semi_batch_ODE.m
constrolled_feed_semi_batch_ODE.m
```

Database

The kinetic and thermodynamic parameters for specific combinations of monomers (e.g. BMA-Styrene) are contained inside istances of the `BinaryCopolymerizationSystem` class, which are saved inside the `Database.mat` file. In order to make changes to the database one must modify the script `Database.m` and run it in order to apply those changes to `Database.mat`. `BinaryCopolymerizationSystem` contains the `pseudo_kinetic_constants` method which evaluates the kinetic constants used in the governing equations of the reactor with the pseudo-homogeneous approach.

Semi-batch reactor model

`semi_batch_ODE` evaluates the derivatives corresponding to its 11×11 system of governing equations. The inlet feed rates `Fin` accepted by this function are constant values. In order to use feed laws in which `Fin` changes over time it is suggested to use an external function that inputs the correct time-dependant values to `semi_batch_ODE` at each integration step. Examples of such functions are `constant_feed_semi_batch_ODE` and `controlled_feed_semi_batch_ODE`.

Auxiliary functions

- `Mayo_Lewis_equation`: returns the results of the Mayo-Lewis equation for the given set of monomeric compositions and reactive ratios.
- `conversion_target_event`: is used to stop the integration when the desired conversion value is reached.
- `CLD_and_MWD_reconstruction`: is used to draw the chain length and mass weight distributions from the first three moments of the chain length distribution.
- `logspacing`: returns an equally-spaced vector for logaritmic plots.

Script structure

The provided template scripts have a similar structure, in which the all caps titles denote the sections that should be edited by the user:

0. USER OPTIONS: contains the main parameters set by the user, such as the monomer combination, temperature, simulation time and other input/output options for the script.
1. Load system properties: loads the properties of the chosen comonomer composition from the database.
2. DESIRED PRODUCT SPECIFICATIONS AND FEED STRATEGY: in this section the initial conditions in the reactor and parameters relative to the feed strategies can be defined by the user.
3. ODE FUNCTION AND INITIAL CONDITIONS: here the user must define the ode function that will be integrated in the following section together with its initial conditions.
4. Numerical integration: the ode function is integrated (usually with `ode23s`) and the results are unpacked.
5. Post-Processing: plots etc...
6. Mayo-Lewis GIF: a .gif image showing the evolution of istantaneous polymer composition with respect to conversion is created. The process, which might take a few seconds, can be activated by setting `MAKEGIF = 1` in the USER OPTIONS section. When finished the .gif file is opened in windows' default image viewer. The .gif file must be closed when running the script in order to avoid runtime errors.
7. Save all figures: saves all the figures created by the Post-Processing section to the current directory. The process can be activated by setting `SAVEFIGURES = 1` in the USER OPTIONS section.
8. Done: signals the end of the script execution.

Examples

A few example scripts are provided which investigate various feed strategies for a semi-batch reactor:

- `BATCH_OPERATION.m`: BMA-Styrene batch copolymerization;
- `BATCH_OPERATION_HOMOPOLYMERIZATION.m`: BMA batch homopolymerization;
- `BATCH_OPERATION_DEPROPAGATION_COMPARISON.m`: comparison between batch copolymerization with and without considering BMA depropagation;
- `SEMI_BATCH_OPERATION.m`: BMA-Styrene copolymerization in a semi-batch reaction with constant feed rate and ratio;
- `SEMI_BATCH_OPERATION_FEED_TIME_COMPARISON.m`: comparison between different feed rates, from fast-feed to starved-feed regime;
- `CONTROLLED_SEMI_BATCH_OPERATION.m`: BMA-Styrene copolymerization in a semi-batch reaction with constant feed and PI-controlled feed ratio.

Resources

Literature about BMA-Styrene copolymerization:

- BMA-Styrene kinetic study
- BMA-Styrene semi-batch copolymerization
- BMA-BA semi-batch copolymerization
- Semi-batch copolymerization control

Great cheat-sheet LaTeX template: A quick guide to LaTeX

Matteo Perego - MathWorks File Exchange profile