



BPL_YEAST_AIR_Fedbatch script with PyFMI ver 2.9.8

The key library PyFMI v2.9.8 is installed.

After the installation a small application BPL_YEAST_AIR_Fedbatch is loaded and run.
You can continue with this example if you like.

```
In [ ]: !lsb_release -a # Actual VM Ubuntu version used by Google
```

```
No LSB modules are available.  
Distributor ID: Ubuntu  
Description:    Ubuntu 20.04.5 LTS  
Release:        20.04  
Codename:       focal
```

```
In [ ]: %env PYTHONPATH=
```

```
env: PYTHONPATH=
```

```
In [ ]: !wget https://repo.anaconda.com/miniconda/Miniconda3-py38_22.11.1-1-Linux  
!chmod +x Miniconda3-py38_22.11.1-1-Linux-x86_64.sh  
!bash ./Miniconda3-py38_22.11.1-1-Linux-x86_64.sh -b -f -p /usr/local  
import sys  
sys.path.append('/usr/local/lib/python3.8/site-packages/')
```

```
--2023-02-24 06:55:13-- https://repo.anaconda.com/miniconda/Miniconda3-  
py38_22.11.1-1-Linux-x86_64.sh  
Resolving repo.anaconda.com (repo.anaconda.com)... 104.16.130.3, 104.16.  
131.3, 2606:4700::6810:8303, ...  
Connecting to repo.anaconda.com (repo.anaconda.com)|104.16.130.3|:443...  
connected.  
HTTP request sent, awaiting response... 200 OK  
Length: 64630241 (62M) [application/x-sh]  
Saving to: 'Miniconda3-py38_22.11.1-1-Linux-x86_64.sh'
```

```
Miniconda3-py38_22. 100%[=====>] 61.64M 168MB/s in  
0.4s
```

```
2023-02-24 06:55:13 (168 MB/s) - 'Miniconda3-py38_22.11.1-1-Linux-x86_6  
4.sh' saved [64630241/64630241]
```

```
PREFIX=/usr/local  
Unpacking payload ...
```

```
Installing base environment...
```

```
Downloading and Extracting Packages
```

```
Downloading and Extracting Packages
```

```
Preparing transaction: done  
Executing transaction: done  
installation finished.
```

```
In [ ]: !conda update -n base -c defaults conda --yes
```

Collecting package metadata (current_repodata.json): done
Solving environment: done

Package Plan

environment location: /usr/local

added / updated specs:
- conda

The following packages will be downloaded:

package	build	
-----	-----	
ca-certificates-2023.01.10	h06a4308_0	120 KB
conda-23.1.0	py38h06a4308_0	942 KB
conda-package-handling-2.0.2	py38h06a4308_0	267 KB
conda-package-streaming-0.7.0	py38h06a4308_0	26 KB
cryptography-38.0.4	py38h9ce1e76_0	1.4 MB
ncurses-6.4	h6a678d5_0	914 KB
openssl-1.1.1t	h7f8727e_0	3.7 MB
sqlite-3.40.1	h5082296_0	1.2 MB
urllib3-1.26.14	py38h06a4308_0	196 KB
xz-5.2.10	h5eee18b_1	429 KB
zstandard-0.19.0	py38h5eee18b_0	474 KB
-----	-----	
Total:		9.6 MB

The following NEW packages will be INSTALLED:

conda-package-str~ pkgs/main/linux-64::conda-package-streaming-0.7.0-py38h06a4308_0
zstandard pkgs/main/linux-64::zstandard-0.19.0-py38h5eee18b_0

The following packages will be UPDATED:

ca-certificates 2022.10.11-h06a4308_0 --> 2023.01.10-h06a4308_0
conda 22.11.1-py38h06a4308_4 --> 23.1.0-py38h06a4308_0
conda-package-han~ 1.9.0-py38h5eee18b_1 --> 2.0.2-py38h06a4308_0
cryptography 38.0.1-py38h9ce1e76_0 --> 38.0.4-py38h9ce1e76_0
ncurses 6.3-h5eee18b_3 --> 6.4-h6a678d5_0
openssl 1.1.1s-h7f8727e_0 --> 1.1.1t-h7f8727e_0
sqlite 3.40.0-h5082296_0 --> 3.40.1-h5082296_0
urllib3 1.26.13-py38h06a4308_0 --> 1.26.14-py38h06a4308_0
xz 5.2.8-h5eee18b_0 --> 5.2.10-h5eee18b_1

Downloading and Extracting Packages
xz-5.2.10 | 429 KB | : 0% 0/1 [00:00<?, ?it/s]

conda-23.1.0	942 KB	:	0% 0/1	[00:00<?, ?it/s]
zstandard-0.19.0	474 KB	:	0% 0/1	[00:00<?, ?it/s]
urllib3-1.26.14	196 KB	:	0% 0/1	[00:00<?, ?it/s]
conda-package-handli	267 KB	:	0% 0/1	[00:00<?, ?it/s]
ncurses-6.4	914 KB	:	0% 0/1	[00:00<?, ?it/s]
sqlite-3.40.1	1.2 MB	:	0% 0/1	[00:00<?, ?it/s]
ca-certificates-2023	120 KB	:	0% 0/1	[00:00<?, ?it/s]
conda-package-stream	26 KB	:	0% 0/1	[00:00<?, ?it/s]
cryptography-38.0.4	1.4 MB	:	0% 0/1	[00:00<?, ?it/s]
xz-5.2.10	429 KB	:	19% 0.18633724038004426/1	[00:00<00:00, 1.78it/s]
urllib3-1.26.14	196 KB	:	8% 0.0816656116198043/1	[00:00<00:01, 1.23s/it]

conda-23.1.0 | 942 KB | : 2% 0.016977341093890375/1 [00:00<00:06, 6.60s/it]

zstandard-0.19.0 | 474 KB | : 3% 0.033766335474643305/1 [00:00<00:03, 3.57s/it]

conda-package-handli | 267 KB | : 6% 0.05994701947985423/1 [00:00<00:01, 2.00s/it]

ncurses-6.4 | 914 KB | : 2% 0.01750655534161504/1 [00:00<00:09, 9.45s/it]

sqlite-3.40.1 | 1.2 MB | : 1% 0.013408406442320282/1 [00:00<00:11, 11.85s/it]

conda-package-stream | 26 KB | : 61% 0.6093197961991893/1 [00:00<00:00, 3.25it/s]

cryptography-38.0.4 | 1.4 MB | : 1% 0.011144350078426731/1 [00:00<00:17, 17.90s/it]

ca-certificates-2023 | 120 KB | : 13% 0.13346258176456693/1 [00:00<00:01, 1.83s/it]

xz-5.2.10 | 429 KB | : 100% 1.0/1 [00:00<00:00, 3.15it/s]

```

urllib3-1.26.14      | 196 KB      | : 100% 1.0/1 [00:00<00:00, 2.66it/s]

urllib3-1.26.14      | 196 KB      | : 100% 1.0/1 [00:00<00:00, 2.66it/s]
zstandard-0.19.0     | 474 KB      | : 100% 1.0/1 [00:00<00:00, 2.39it/s]
zstandard-0.19.0     | 474 KB      | : 100% 1.0/1 [00:00<00:00, 2.39it/s]


conda-package-handli | 267 KB      | : 100% 1.0/1 [00:00<00:00, 2.21it/s]


conda-package-handli | 267 KB      | : 100% 1.0/1 [00:00<00:00, 2.21it/s]
conda-23.1.0         | 942 KB      | : 100% 1.0/1 [00:00<00:00, 1.71it/s]
conda-23.1.0         | 942 KB      | : 100% 1.0/1 [00:00<00:00, 1.71it/s]


ncurses-6.4          | 914 KB      | : 100% 1.0/1 [00:00<00:00, 1.10it/s]


ncurses-6.4          | 914 KB      | : 100% 1.0/1 [00:00<00:00, 1.10it/s]


sqlite-3.40.1         | 1.2 MB      | : 100% 1.0/1 [00:01<00:00, 1.04it/s]


sqlite-3.40.1         | 1.2 MB      | : 100% 1.0/1 [00:01<00:00, 1.04it/s]


conda-package-stream | 26 KB       | : 100% 1.0/1 [00:01<00:00, 1.21s/it]


conda-package-stream | 26 KB       | : 100% 1.0/1 [00:01<00:00, 1.21s/it]

```

ca-certificates-2023 | 120 KB | : 100% 1.0/1 [00:01<00:00, 1.05s/it]

ca-certificates-2023 | 120 KB | : 100% 1.0/1 [00:01<00:00, 1.05s/it]

cryptography-38.0.4 | 1.4 MB | : 100% 1.0/1 [00:01<00:00, 1.14s/it]

cryptography-38.0.4 | 1.4 MB | : 100% 1.0/1 [00:01<00:00, 1.14s/it]

openssl-1.1.1t | 3.7 MB | : 100% 1.0/1 [00:01<00:00, 1.25s/it]

```
Preparing transaction: done  
Verifying transaction: done  
Executing transaction: done
```

```
In [ ]: !conda --version  
        !python --version
```

```
conda 23.1.0  
Python 3.8.15
```

```
In [ ]: !conda install -c conda-forge pyfmi --yes # Install the key package
```


Collecting package metadata (current_repodata.json): done
Solving environment: done

Package Plan

environment location: /usr/local

added / updated specs:

- pyfmi

The following packages will be downloaded:

package	build		
-----	-----		
_libgcc_mutex-0.1	conda_forge	3 KB	conda-
forge			
_openmp_mutex-4.5	2_kmp_llvm	6 KB	conda-
forge			
appdirs-1.4.4	pyh9f0ad1d_0	13 KB	conda-
forge			
assimulo-3.3	py38h71f17ff_1	2.4 MB	conda-
forge			
ca-certificates-2022.12.7	ha878542_0	143 KB	conda-
forge			
certifi-2022.12.7	pyhd8ed1ab_0	147 KB	conda-
forge			
fmilib-2.4.1	h27087fc_0	545 KB	conda-
forge			
gmp-6.2.1	h58526e2_0	806 KB	conda-
forge			
icu-58.2	hf484d3e_1000	22.6 MB	conda-
forge			
libblas-3.9.0	16_linux64_openblas	13 KB	cond
a-forge			
libcbblas-3.9.0	16_linux64_openblas	13 KB	cond
a-forge			
libgcc-ng-12.2.0	h65d4601_19	931 KB	conda-
forge			
libgfortran-ng-12.2.0	h69a702a_19	22 KB	conda-
forge			
libgfortran5-12.2.0	h337968e_19	1.8 MB	conda-
forge			
liblapack-3.9.0	16_linux64_openblas	13 KB	cond
a-forge			
libopenblas-0.3.21	pthread_h78a6416_3	10.1 MB	cond
a-forge			
libstdcxx-ng-12.2.0	h46fd767_19	4.3 MB	conda-
forge			
libxml2-2.9.14	h74e7548_0	718 KB	
libxslt-1.1.35	h4e12654_0	453 KB	
llvm-openmp-14.0.6	h9e868ea_0	4.4 MB	
lxml-4.9.1	py38h1edc446_0	1.3 MB	
metis-5.1.0	h58526e2_1006	4.1 MB	conda-
forge			
mpfr-4.1.0	h9202a9a_1	2.6 MB	conda-
forge			
numpy-1.24.2	py38h10c12cc_0	6.3 MB	conda-
forge			
openssl-1.1.1t	h0b41bf4_0	1.9 MB	conda-

forge				
packaging-23.0		pyhd8ed1ab_0	40 KB	conda-
forge				
pooch-1.6.0		pyhd8ed1ab_0	44 KB	conda-
forge				
pyfmi-2.9.8		py38h26c90d9_1	12.7 MB	conda-
forge				
python_abi-3.8		2_cp38	4 KB	conda-
forge				
scipy-1.10.1		py38h10c12cc_0	23.6 MB	conda-
forge				
suitesparse-5.10.1		hd8046ac_0	2.4 MB	conda-
forge				
sundials-6.4.1		h89a52a3_0	1.2 MB	conda-
forge				
tbb-2020.2		h4bd325d_4	1.5 MB	conda-
forge				

Total:			106.7 MB	

The following NEW packages will be INSTALLED:

appdirs	conda-forge/noarch::appdirs-1.4.4-pyh9f0ad1d_0
assimulo	conda-forge/linux-64::assimulo-3.3-py38h71f17ff_1
fmilib	conda-forge/linux-64::fmilib-2.4.1-h27087fc_0
gmp	conda-forge/linux-64::gmp-6.2.1-h58526e2_0
icu	conda-forge/linux-64::icu-58.2-hf484d3e_1000
libblas	conda-forge/linux-64::libblas-3.9.0-16_linux64_open
blas	
libcbblas	conda-forge/linux-64::libcbblas-3.9.0-16_linux64_ope
nblas	
libgfortran-ng	conda-forge/linux-64::libgfortran-ng-12.2.0-h69a702
a_19	
libgfortran5	conda-forge/linux-64::libgfortran5-12.2.0-h337968e_
19	
liblapack	conda-forge/linux-64::liblapack-3.9.0-16_linux64_op
enblas	
libopenblas	conda-forge/linux-64::libopenblas-0.3.21-pthreads_h
78a6416_3	
libxml2	pkgs/main/linux-64::libxml2-2.9.14-h74e7548_0
libxslt	pkgs/main/linux-64::libxslt-1.1.35-h4e12654_0
llvm-openmp	pkgs/main/linux-64::llvm-openmp-14.0.6-h9e868ea_0
lxml	pkgs/main/linux-64::lxml-4.9.1-py38h1edc446_0
metis	conda-forge/linux-64::metis-5.1.0-h58526e2_1006
mpfr	conda-forge/linux-64::mpfr-4.1.0-h9202a9a_1
numpy	conda-forge/linux-64::numpy-1.24.2-py38h10c12cc_0
packaging	conda-forge/noarch::packaging-23.0-pyhd8ed1ab_0
pooch	conda-forge/noarch::pooch-1.6.0-pyhd8ed1ab_0
pyfmi	conda-forge/linux-64::pyfmi-2.9.8-py38h26c90d9_1
python_abi	conda-forge/linux-64::python_abi-3.8-2_cp38
scipy	conda-forge/linux-64::scipy-1.10.1-py38h10c12cc_0
suitesparse	conda-forge/linux-64::suitesparse-5.10.1-hd8046ac_0
sundials	conda-forge/linux-64::sundials-6.4.1-h89a52a3_0
tbb	conda-forge/linux-64::tbb-2020.2-h4bd325d_4

The following packages will be REMOVED:

libgomp-11.2.0-h1234567_1

The following packages will be UPDATED:

```
libgcc-ng          pkgs/main::libgcc-ng-11.2.0-h1234567_1 --> conda-forge::libgcc-ng-12.2.0-h65d4601_19
libstdcxx-ng       pkgs/main::libstdcxx-ng-11.2.0-h12345~ --> conda-forge::libstdcxx-ng-12.2.0-h46fd767_19
```

The following packages will be SUPERSEDED by a higher-priority channel:

```
_libgcc_mutex      pkgs/main::_libgcc_mutex-0.1-main --> conda-forge::_libgcc_mutex-0.1-conda_forge
_openmp_mutex      pkgs/main::_openmp_mutex-5.1-1_gnu --> conda-forge::_openmp_mutex-4.5-2_kmp_llvm
ca-certificates    pkgs/main::ca-certificates-2023.01.10~ --> conda-forge::ca-certificates-2022.12.7-ha878542_0
certifi            pkgs/main/linux-64::certifi-2022.12.7~ --> conda-forge/noarch::certifi-2022.12.7-pyhd8ed1ab_0
openssl            pkgs/main::openssl-1.1.1t-h7f8727e_0 --> conda-forge::openssl-1.1.1t-h0b41bf4_0
```

Downloading and Extracting Packages

```
libstdcxx-ng-12.2.0 | 4.3 MB | : 0% 0/1 [00:00<?, ?it/s]
libgfortran-ng-12.2. | 22 KB | : 0% 0/1 [00:00<?, ?it/s]
```

```
assimulo-3.3 | 2.4 MB | : 0% 0/1 [00:00<?, ?it/s]
```

```
metis-5.1.0 | 4.1 MB | : 0% 0/1 [00:00<?, ?it/s]
```

```
packaging-23.0 | 40 KB | : 0% 0/1 [00:00<?, ?it/s]
```

```
gmp-6.2.1 | 806 KB | : 0% 0/1 [00:00<?, ?it/s]
```

```
pyfmi-2.9.8 | 12.7 MB | : 0% 0/1 [00:00<?, ?it/s]
```

```
suitesparse-5.10.1 | 2.4 MB | : 0% 0/1 [00:00<?, ?it/s]
```

```
tbb-2020.2 | 1.5 MB | : 0% 0/1 [00:00<?, ?it/s]
```

sundials-6.4.1 | 1.2 MB | : 0% 0/1 [00:00<?, ?it/s]

liblapack-3.9.0 | 13 KB | : 0% 0/1 [00:00<?, ?it/s]

libxml2-2.9.14 | 718 KB | : 0% 0/1 [00:00<?, ?it/s]

ca-certificates-2022 | 143 KB | : 0% 0/1 [00:00<?, ?it/s]

appdirs-1.4.4 | 13 KB | : 0% 0/1 [00:00<?, ?it/s]

pooch-1.6.0 | 44 KB | : 0% 0/1 [00:00<?, ?it/s]

fmilib-2.4.1 | 545 KB | : 0% 0/1 [00:00<?, ?it/s]

numpy-1.24.2 | 6.3 MB | : 0% 0/1 [00:00<?, ?it/s]

llvm-openmp-14.0.6 | 4.4 MB | : 0% 0/1 [00:00<?, ?it/s]

_libgcc_mutex-0.1 | 3 KB | : 0% 0/1 [00:00<?, ?it/s]

... (more hidden) ...

libstdcxx-ng-12.2.0 | 4.3 MB | : 0% 0.003642462432659798/1 [00:00<00:33, 33.42s/it]
libgfortran-ng-12.2. | 22 KB | : 72% 0.7159587484705471/1 [00:00<00:00, 5.87it/s]

metis-5.1.0 | 4.1 MB | : 0% 0.003823948974180876/1 [00:00<00:33, 33.68s/it]

gmp-6.2.1 | 806 KB | : 2% 0.019840539414665338/1 [00:00<00:06, 6.99s/it]
assimulo-3.3 | 2.4 MB | : 1% 0.006554934584681441/1 [00:00<00:23, 23.45s/it]

libstdcxx-ng-12.2.0 | 4.3 MB | : 30% 0.29503945704544365/1 [00:00<00:00, 1.53it/s]

packaging-23.0	40 KB	: 100% 1.0/1 [00:00<00:00, 4.45it/s]
packaging-23.0	40 KB	: 100% 1.0/1 [00:00<00:00, 4.45it/s]
metis-5.1.0	4.1 MB	: 34% 0.34033145870209797/1 [00:00<00:00, 1.67it/s]
assimulo-3.3	2.4 MB	: 45% 0.45229048634301944/1 [00:00<00:00, 2.15it/s]
libgfortran-ng-12.2.	22 KB	: 100% 1.0/1 [00:00<00:00, 5.87it/s]
pyfmi-2.9.8	12.7 MB	: 14% 0.1439087057526982/1 [00:00<00:01, 1.57s/it]
libstdcxx-ng-12.2.0	4.3 MB	: 73% 0.7284924865319596/1 [00:00<00:00, 2.69it/s]
metis-5.1.0	4.1 MB	: 73% 0.7341982030427282/1 [00:00<00:00, 2.59it/s]
tbb-2020.2	1.5 MB	: 1% 0.01070822377730241/1 [00:00<00:32, 32.68s/it]
pyfmi-2.9.8	12.7 MB	: 30% 0.30380726770014066/1 [00:00<00:00, 1.01it/s]
suitesparse-5.10.1	2.4 MB	: 75% 0.749963082182048/1 [00:00<00:00, 2.45it/s]

liblapack-3.9.0 | 13 KB | : 100% 1.0/1 [00:00<00:00, 2.14it/s]

ca-certificates-2022 | 143 KB | : 11% 0.11222532741520083/1 [00:00<00:03, 4.22s/it]

sundials-6.4.1 | 1.2 MB | : 1% 0.013387928801451884/1 [00:00<00:35, 35.50s/it]

pyfmi-2.9.8 | 12.7 MB | : 44% 0.43787606194838086/1 [00:00<00:00, 1.12it/s]

appdirs-1.4.4 | 13 KB | : 100% 1.0/1 [00:00<00:00, 2.00it/s]

pooch-1.6.0 | 44 KB | : 37% 0.36539619527643347/1 [00:00<0
0:00, 1.40s/it]

numpy-1.24.2 | 6.3 MB | : 0% 0.00246386425166665/1 [00:00<0
3:40, 221.33s/it]

fmilib-2.4.1 | 545 KB | : 3% 0.029341289483769524/1 [00:00<
00:18, 19.07s/it]

pyfmi-2.9.8 | 12.7 MB | : 63% 0.6322143141614263/1 [00:00<0
0:00, 1.39it/s]

llvm-openmp-14.0.6 | 4.4 MB | : 0% 0.0035718910660429226/1 [00:00<02:51, 171.73s/it]

libxml2-2.9.14 | 718 KB | : 2% 0.022280425482148734/1 [00:00<00:27, 27.82s/it]

_libgcc_mutex-0.1 | 3 KB | : 100% 1.0/1 [00:00<00:00, 1.61it/s]

numpy-1.24.2 | 6.3 MB | : 28% 0.2759527961866648/1 [00:00<00:01, 1.75s/it]

... (more hidden) ...

pyfmi-2.9.8 | 12.7 MB | : 82% 0.8216326106222427/1 [00:00<0
0:00, 1.56it/s]

llvm-openmp-14.0.6 | 4.4 MB | : 37% 0.371476670868464/1 [00:00<00:
00, 1.44s/it]

numpy-1.24.2 | 6.3 MB | : 50% 0.5026283073399965/1 [00:00<0
0:00, 1.04s/it]

... (more hidden) ...

pyfmi-2.9.8 | 12.7 MB | : 99% 0.9852211393838569/1 [00:00<0
0:00, 1.54it/s]

llvm-openmp-14.0.6 | 4.4 MB | : 74% 0.742953341736928/1 [00:00<00:
00, 1.33it/s]

numpy-1.24.2 | 6.3 MB | : 75% 0.7539424610099948/1 [00:00<0
0:00, 1.34it/s]

... (more hidden) ...

... (more hidden) ...

... (more hidden) ...

... (more hidden) ...

gmp-6.2.1	806 KB	: 100% 1.0/1 [00:01<00:00, 1.22s/it]
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gmp-6.2.1	806 KB	: 100% 1.0/1 [00:01<00:00, 1.22s/it]
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... (more hidden) ...

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... (more hidden) ...

... (more hidden) ...

assimulo-3.3	2.4 MB	: 100% 1.0/1 [00:02<00:00, 2.37s/it]
libstdcxx-ng-12.2.0	4.3 MB	: 100% 1.0/1 [00:02<00:00, 2.69it/s]
suitesparse-5.10.1	2.4 MB	: 100% 1.0/1 [00:02<00:00, 2.45it/s]
tbb-2020.2	1.5 MB	: 100% 1.0/1 [00:03<00:00, 3.23s/it]

tbb-2020.2 | 1.5 MB | : 100% 1.0/1 [00:03<00:00, 3.23s/it]

liblapack-3.9.0 | 13 KB | : 100% 1.0/1 [00:03<00:00, 2.14it/s]

ca-certificates-2022 | 143 KB | : 100% 1.0/1 [00:03<00:00, 3.32s/it]

ca-certificates-2022 | 143 KB | : 100% 1.0/1 [00:03<00:00, 3.32s/it]

appdirs-1.4.4 | 13 KB | : 100% 1.0/1 [00:03<00:00, 2.00it/s]

pooch-1.6.0 | 44 KB | : 100% 1.0/1 [00:03<00:00, 3.65s/it]

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sundials-6.4.1 | 1.2 MB | : 100% 1.0/1 [00:03<00:00, 3.79s/it]

sundials-6.4.1 | 1.2 MB | : 100% 1.0/1 [00:03<00:00, 3.79s/it]

fmilib-2.4.1 | 545 KB | : 100% 1.0/1 [00:04<00:00, 3.97s/it]

fmilib-2.4.1 | 545 KB | : 100% 1.0/1 [00:04<00:00, 3.97s/it]

_libgcc_mutex-0.1 | 3 KB | : 100% 1.0/1 [00:04<00:00, 1.61it/s]

metis-5.1.0 | 4.1 MB | : 100% 1.0/1 [00:04<00:00, 2.59it/s]

libxml2-2.9.14 | 718 KB | : 100% 1.0/1 [00:04<00:00, 4.01s/it]

libxml2-2.9.14 | 718 KB | : 100% 1.0/1 [00:04<00:00, 4.01s/it]

llvm-openmp-14.0.6 | 4.4 MB | : 100% 1.0/1 [00:05<00:00, 1.33it/s]

numpy-1.24.2 | 6.3 MB | : 100% 1.0/1 [00:06<00:00, 8.78s/it]

numpy-1.24.2 | 6.3 MB | : 100% 1.0/1 [00:06<00:00, 8.78s/it]

pyfmi-2.9.8 | 12.7 MB | : 100% 1.0/1 [00:07<00:00, 1.54it/s]

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Preparing transaction: done
Verifying transaction: done
Executing transaction: done

Notes of BPL_YEAST_AIR_Fedbatch

Now specific installation and the run simulations. Start with connecting to Github. Then upload the two files:

- FMU - BPL_YEAST_AIR_Fedbatch_linux_jm_cs.fmu
- Setup-file - BPL_YEAST_AIR_Fedbatch_explore

```
In [ ]: %%bash
git clone https://github.com/janpeter19/BPL_YEAST_AIR_Fedbatch
```

```
Cloning into 'BPL_YEAST_AIR_Fedbatch'...
```

```
In [ ]: %cd BPL_YEAST_AIR_Fedbatch
/content/BPL_YEAST_AIR_Fedbatch
```

BPL_YEAST_AIR_Fedbatch - demo

Author: Jan Peter Axelsson

This notebook demonstrate yeast fedbatch cultivation. We look at impact of changes in the glucose feeding. We also take a look at tuning of the DO-control system. Both liquid- and gasphase are included in the model. The culture growth and metabolism are formulated in relation to the respiratory capacity [1] and the model is expanded to describe also the gas phase as well as the culture heat production [2]. The model was derived mainly from continuous culture data but proved to capture dynamic aspects well of ethanol production and consumption [3].

Interaction with the compiled model as FMU is mainly through the simplified commands: `par()`, `init()`, `newplot()`, `simu()` etc. The last simulation is always available in the workspace and called 'sim_res'. The command `describe()` brings mainly up description information from the actual Modelica code from the FMU but is complemented with information given in the dedicated Python setup-file.

The idea is to demonstrate how simulations and varying conditions can provide some process insight that can support the experimental work. I hope that at the end of this session you are ready to formulate your own questions you want to address with simulations - and you can just go on in this notebook! Just press the field "+Code" in the upper left part of notebook interface and you get a new "cell" where you write your own code. You can copy and paste from cells above using `ctrl-c` and `ctrl-p` as usual and edit

the cell. When you are ready to execute the cell just press the "play button" to the left in the cell or press shift-enter as in "ordinary" Jupyter notebooks.

After a session you may want to save your own notebook. That you can do on your Google Drive account and I refer to Colab instructions for how to do this. It is easy.

Enjoy!

```
In [22]: run -i BPL_YEAST_AIR_Fedbatch_D0control_explore.py
```

Linux - run FMU pre-compiled OpenModelica 1.21.0

Model for bioreactor has been setup. Key commands:

- par() - change of parameters and initial values
- init() - change initial values only
- simu() - simulate and plot
- newplot() - make a new plot
- show() - show plot from previous simulation
- disp() - display parameters and initial values from the last simulation
- describe() - describe culture, broth, parameters, variables with values/units

Note that both disp() and describe() takes values from the last simulation

Brief information about a command by help(), eg help(simu)
Key system information is listed with the command system_info()
<Figure size 944.882x787.402 with 0 Axes>

```
In [23]: %matplotlib inline
plt.rcParams['figure.figsize'] = [36/2.54, 30/2.54]
```

About the process model

We can get information about the process, liquid- and gas-phase by the command describe(). This command can also be used to bring up information about a specific variable or parameter. However, you should use describe() after a simulation to get the values used during the simulation.

```
In [24]: describe('culture'); print(); #describe('liquidphase'); print(); describe('gasphase'); print();
```

Saccharomyces cerevisiae - default parameters for strain H1022

The model of the process has parameters both for culture, gas_liquid_transfer, as well as feeding procedure. The parameters that are available for changes you find by the command disp() and you get a long list and you change by them by command par(). The model has even more parameters in the background but not made available for interaction.

First simulations - adjusting start of substrate feeding

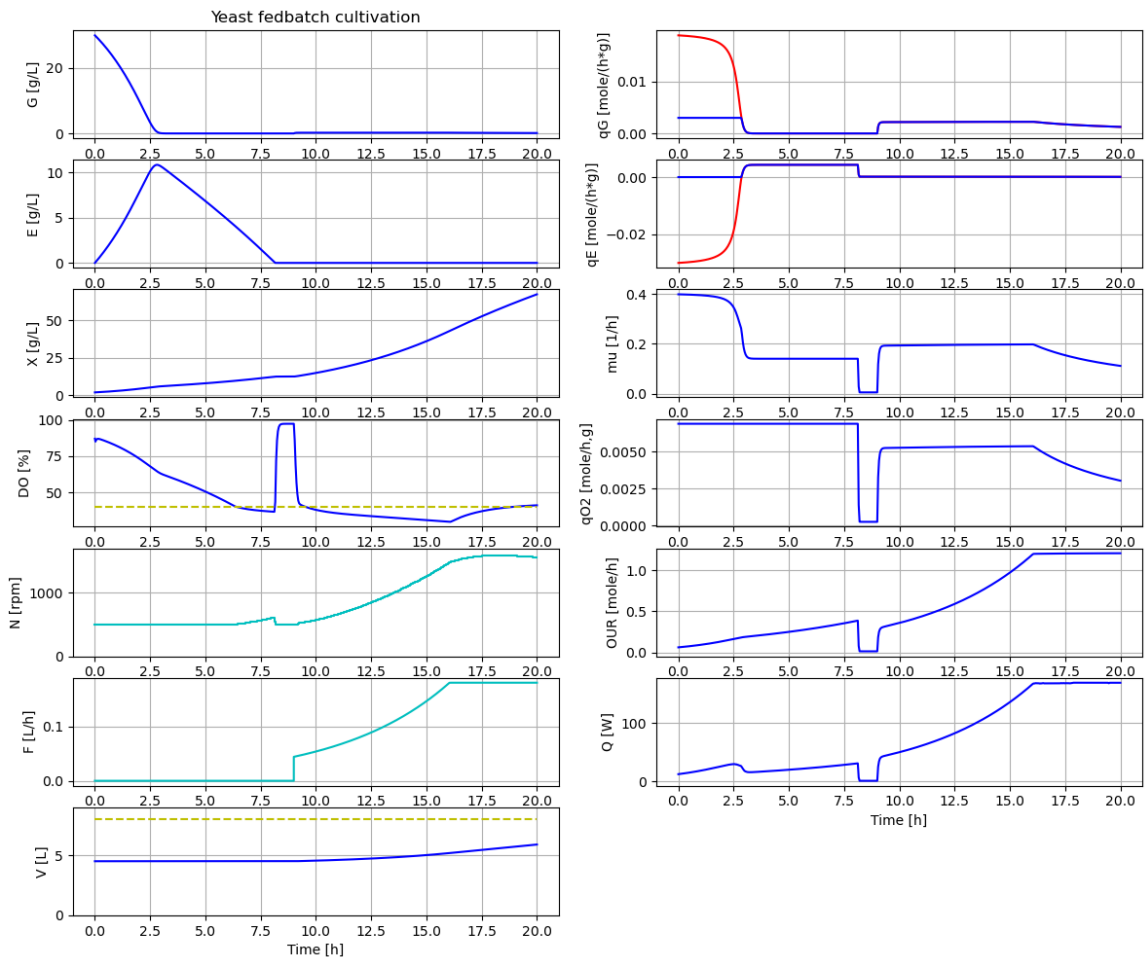
```
In [25]: # Culture parameters and others at default values
par(q02lim=0.0069)

# Process initial conditions
init(V_0=4.5, VG_0=4.5*30, VX_0=4.5*2, VE_0=4.5*0)

# Feed profile
par(t_start=9, F_start=0.044, mu_feed=0.20, F_max=0.18)

# DO-control parameters
par(K=10, Ti=0.5)

# Simulate and plot
newplot(title='Yeast fedbatch cultivation', plotType='Overview')
simu(20)
```



Now we can get value of broth volume as well as the headspace and values are the last ones in the simulation

```
In [26]: describe('bioreactor.V')

Reactor broth volume : 5.892 [ L ]
```

```
In [27]: describe('bioreactor.V_gasphase')
```

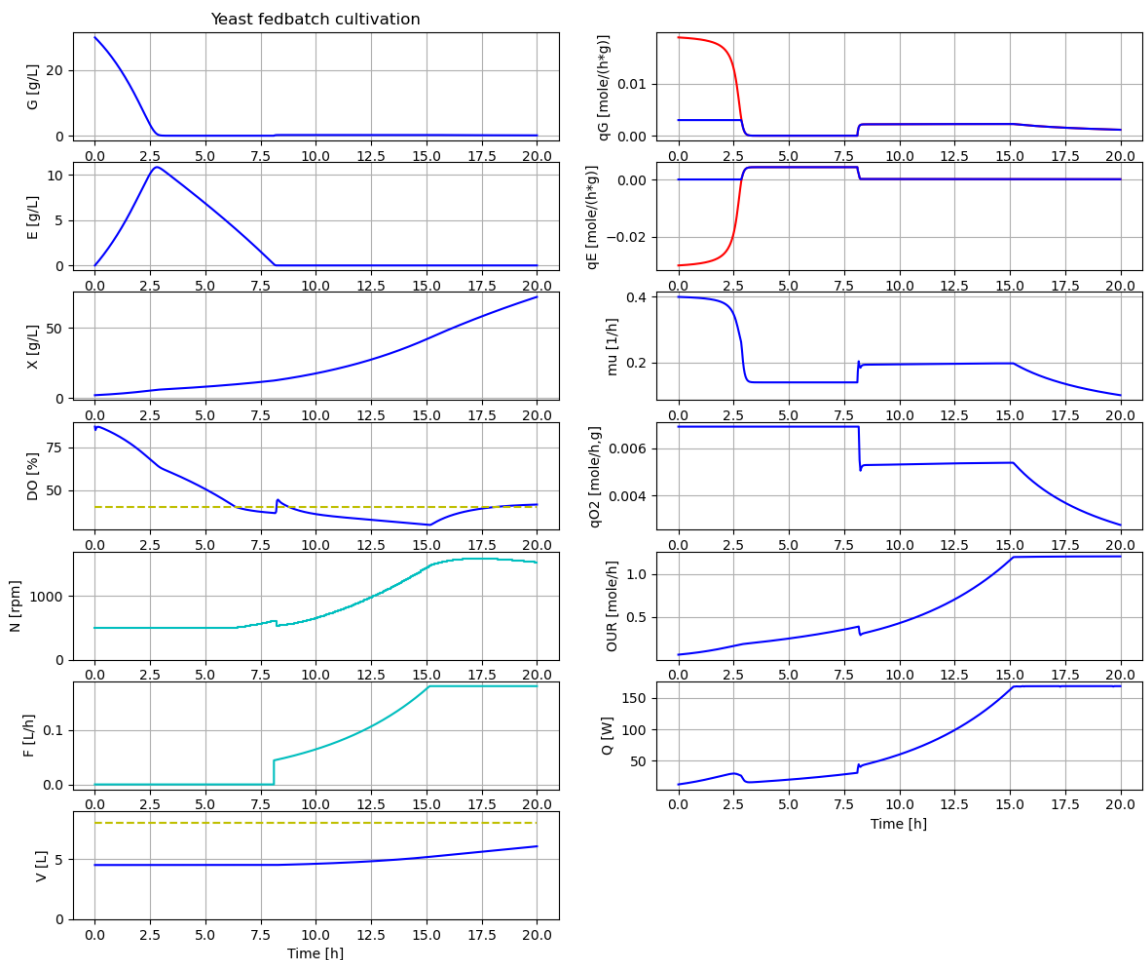
Volume of the gas phase : 2.108 [L]

```
In [28]: # Take a look at the parameters available to adjust the dosage scheme
disp('dosage', decimals=4)
```

```
mu_feed : 0.2
F_0 : 0.0
t_start : 9.0
F_start : 0.044
F_max : 0.18
```

```
In [29]: # Let us start the feeding just after the batch phase has ended and keep
par(t_start=8.1)
```

```
# Simulate and plot
newplot(title='Yeast fedbatch cultivation', plotType='Overview')
simu(20)
```



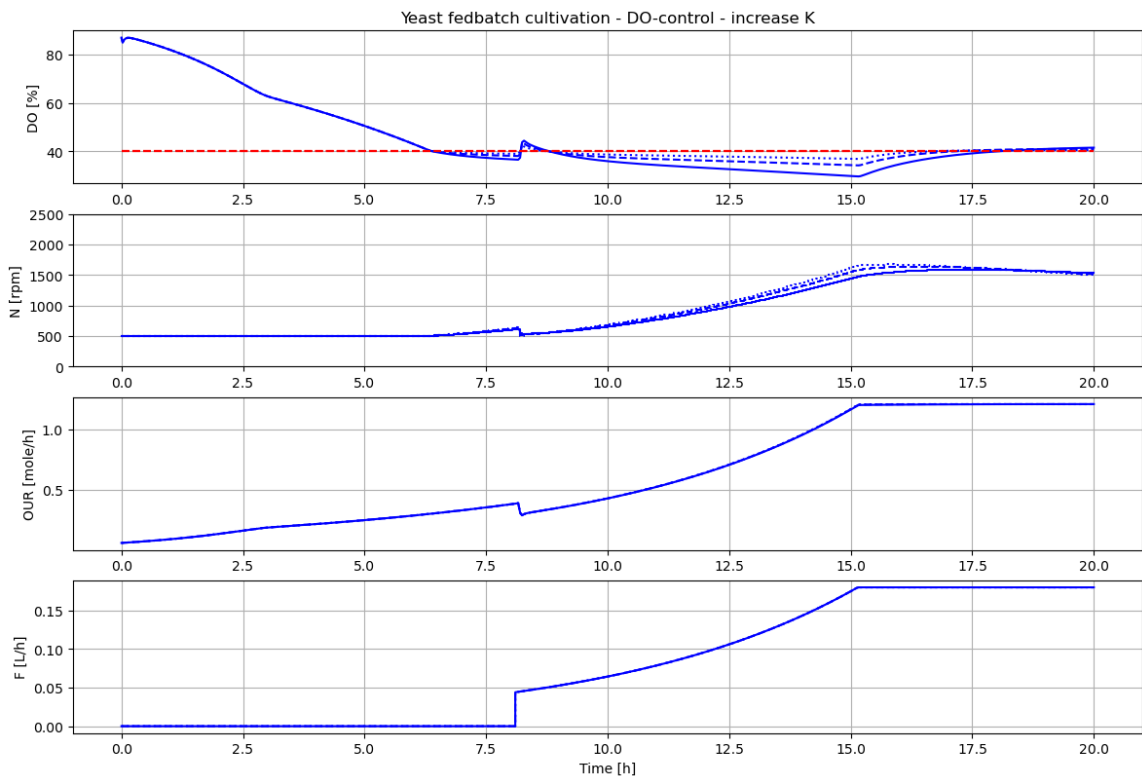
The increase of DO to about 50 % at end of batch phase should be possible to detect easily. This simulation is more realistic and we use these settings from now on.

DO-control - tuning of PI-regulator parameters

Let us focus on the DO-control system and choose a more limited plotType. We study the impact of PI control parameters and see if we can decrease the control error without loosing stability.

```
In [30]: # Let us take a closer look at the DO-control system and try to make cont
newplot(title='Yeast fedbatch cultivation - DO-control - increase K', plo
for value in [10, 20, 40]: par(K=value); simu(20)

# Reset K to the original value
par(K=10)
```



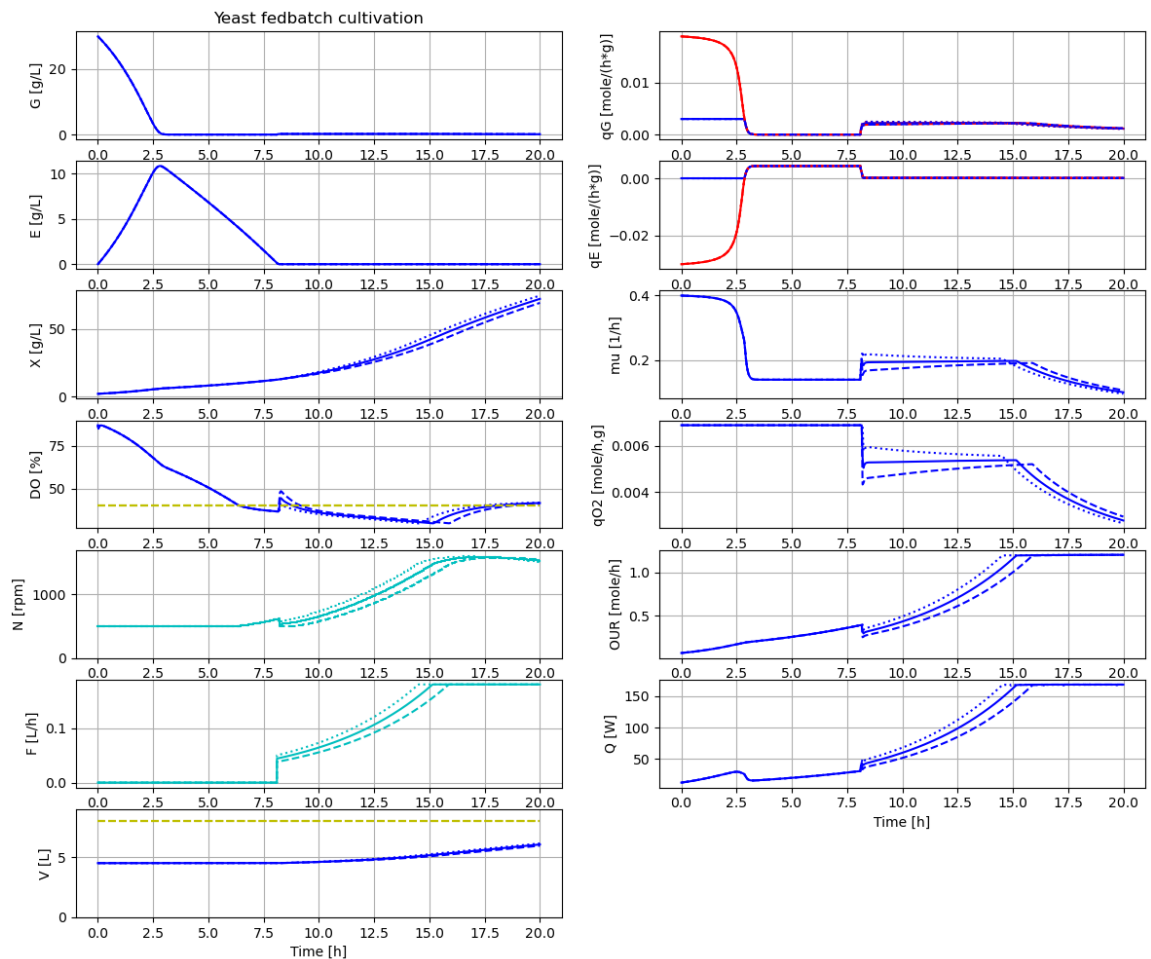
We see that by a higher control gain K the DO-control error get smaller and the stability of the control system is maintained.

Exercise I leave for you to study the impact variation of the T_i -parameter. Just make a new cell below. Then copy and paste the cell above and change parameter to T_i .

Sensitivity to changes in feed-profile

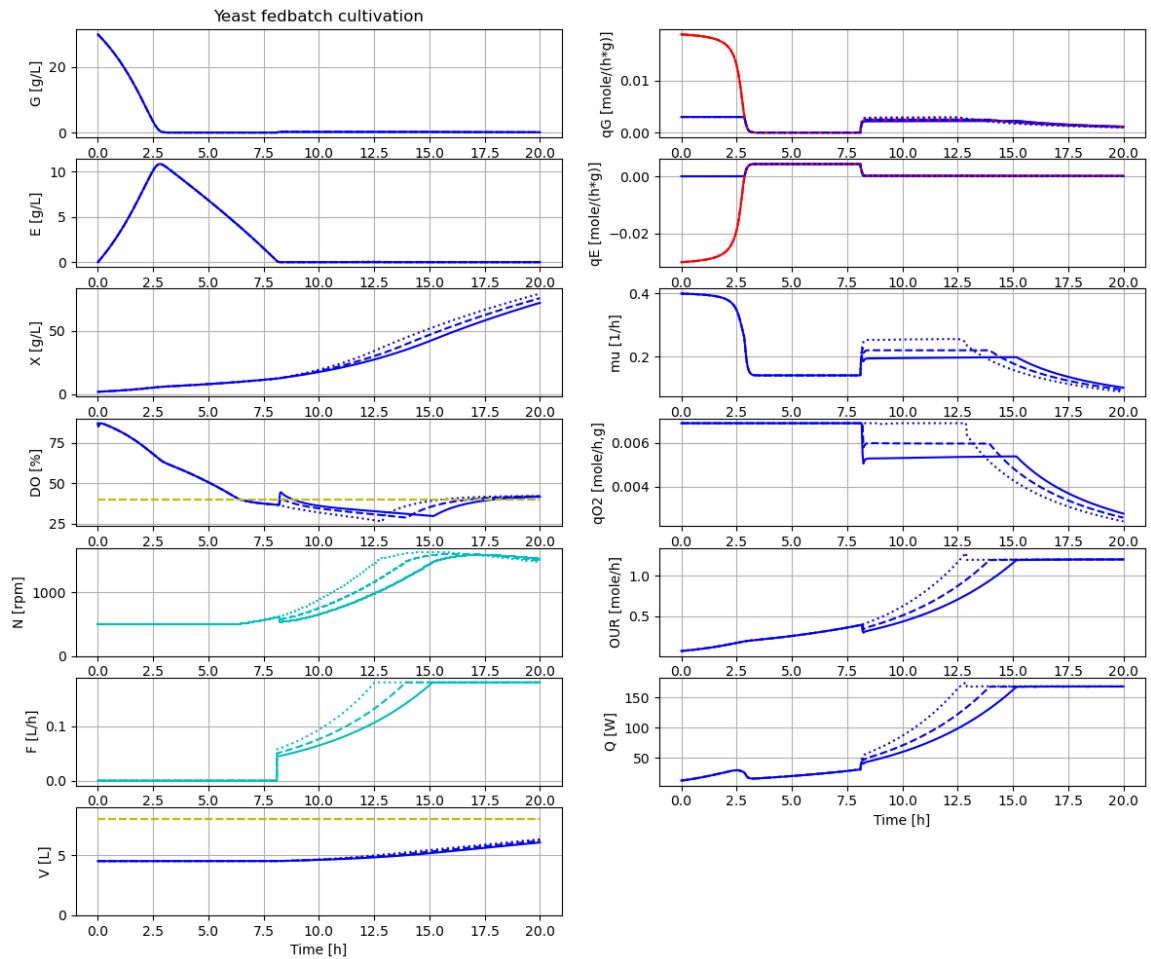
Now, let us focus on investigating impact of changes in the feed-profile. The goal is to increase the produced cell mass without accumulation of by-product ethanol. Simulation can bring some insight into how behaviour of the differen variables change when by-product is formed. This insight can help to interpret experimental results.

```
In [31]: # Let us check the sensitivity to changes in the feed profile design
newplot(title='Yeast fedbatch cultivation', plotType='Overview')
for value in [0.044, 0.038, 0.050]: par(F_start=value); simu(20)
```

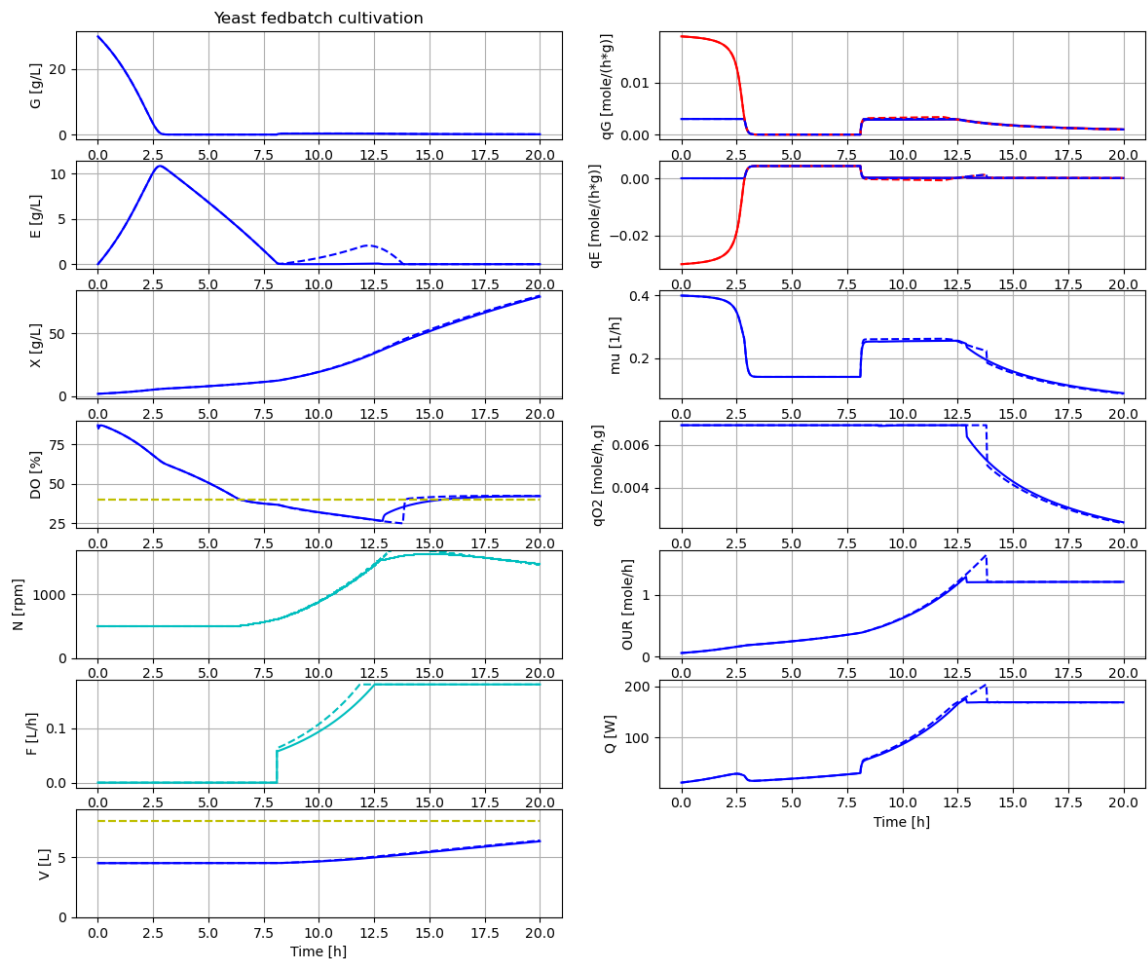


The variation in F_{start} has an impact and we see that the actual growth rate during fedbatch phase do converge to the set growth rate of the feed, but it takes more than 5 hours.

```
In [32]: # Let us investigate a feedprofile that is closer to the maximal capacity
newplot(title='Yeast fedbatch cultivation', plotType='Overview')
par(F_start=0.044, mu_feed=0.20); simu(20)
par(F_start=0.050, mu_feed=0.22); simu(20)
par(F_start=0.057, mu_feed=0.26); simu(20)
```



```
In [33]: # And let us see what happens if the feedprofile exceed the culture capacity
newplot(title='Yeast fedbatch cultivation', plotType='Overview')
par(F_start=0.057, mu_feed=0.26); simu(20)
par(F_start=0.063, mu_feed=0.28); simu(20)
par(F_start=0.044, mu_feed=0.20)
```



Note that with the feedprofile that exceed culture respiratory capacity, ethanol is accumulated during time 8-12.5 hours. When the feedprofile then is constant from time 12.5 hours and on, then the accumulated ethanol is consumed over about an hour. This leads to a higher oxygen demand and heat production during this time. The specific cell growth rate is also slightly higher during this period.

Exercise You can investigate the impact of changing the maximal feedrate F_{\max} . Make sure that the DO level do not get too low.

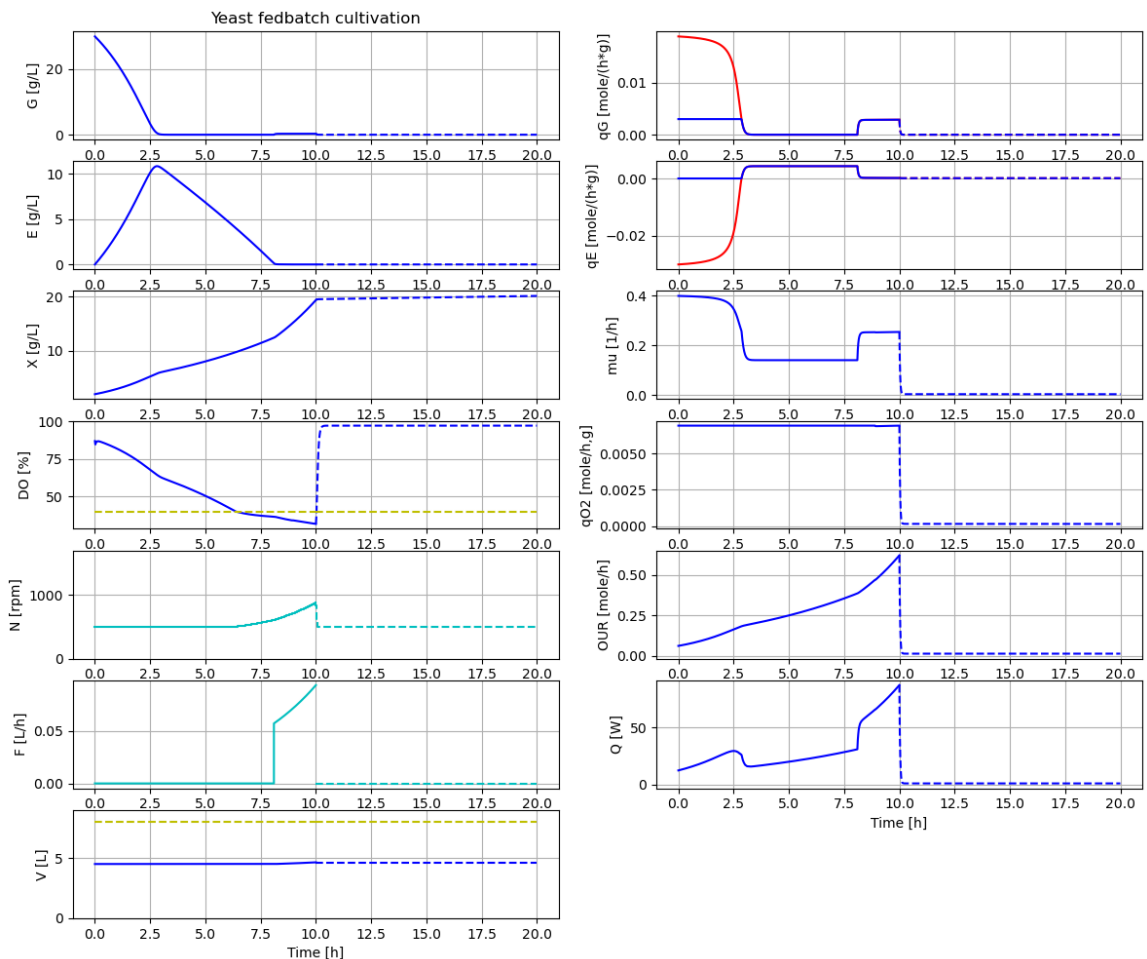
```
In [34]: # Check of simu('cont')
newplot(title='Yeast fedbatch cultivation', plotType='Overview')
par(F_start=0.057, mu_feed=0.26); simu(10)
simu(10,'cont')
```



```

assert          | warning | [/media/sf_Modelica/GitHub/BPL_DEV/BPL/Equ
ipmentLib.mo:141:3-141:90:writable]
|              | |      | The following assertion has been violated
at time 0.000000
|              | |      | ((bioreactor.V_gas_0[4] >= 0.0)) --> "Vari
able violating min constraint: 0.0 <= bioreactor.V_gas_0[4], has value:
-0.0104077"
assert          | warning | [/media/sf_Modelica/GitHub/BPL_DEV/BPL/Equ
ipmentLib.mo:134:3-134:98:writable]
|              | |      | The following assertion has been violated
at time 0.000000
|              | |      | ((bioreactor.x_gas[4] >= 0.0)) --> "Variab
le violating min constraint: 0.0 <= bioreactor.x_gas[4], has value: -0.0
0309757"
assert          | warning | [/media/sf_Modelica/GitHub/BPL_DEV/BPL/Equ
ipmentLib.mo:144:3-144:82:writable]
|              | |      | The following assertion has been violated
at time 0.000000
|              | |      | ((bioreactor.V_gas[4] >= 0.0)) --> "Variab
le violating min constraint: 0.0 <= bioreactor.V_gas[4], has value: -0.0
104077"

```



Make your own diagrams

There are a couple of pre-defined plotType for the application that you make by the command `newplot()`. The command result in a list "diagrams" that describe the commands that make the plot when you call `simu()` or you just want to look at the last simulation again with a changed plotType using `show()`.

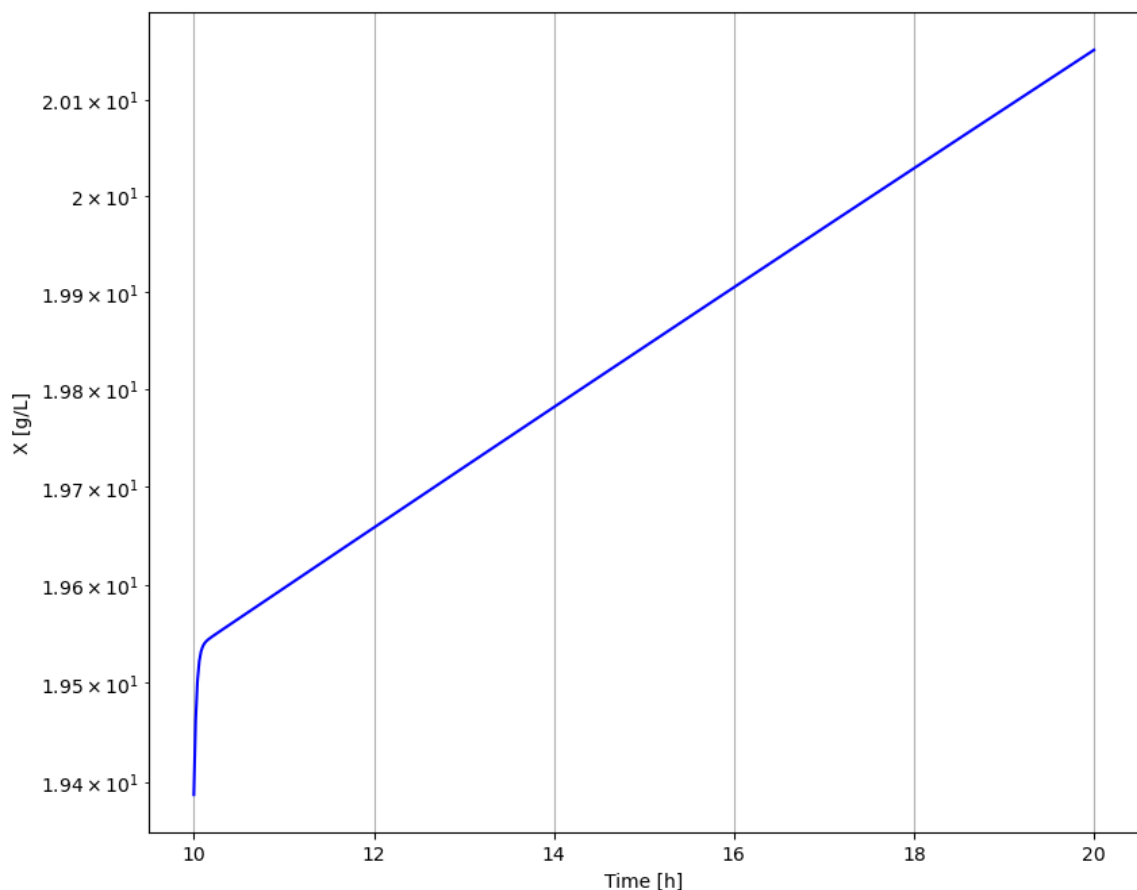
You can also in Jupyter notebook directly define the list "diagrams" and then that will be used for subsequent calls of `simu()` or `show()`. When you have made a diagram that you want to reuse many times you can bring it into the python-setup file and edit the `newplot()` command and add a new `plotType`.

Below a few simple examples that show how to do a diagram directly i the notebook

```
In [35]: # First decrease the diagram size
plt.rcParams['figure.figsize'] = [24/2.54, 20/2.54]

In [36]: # Improvise and make your own diagram - cell concentration in a logarithmic
plt.figure()
ax1 = plt.subplot(1,1,1)
ax1.set_ylabel('X [g/L]')
ax1.set_xlabel('Time [h]')
ax1.grid()

setLines()
diagrams.clear()
diagrams.append("ax1.semilogy(sim_res['time'], sim_res['bioreactor.c[1]'])")
show()
```

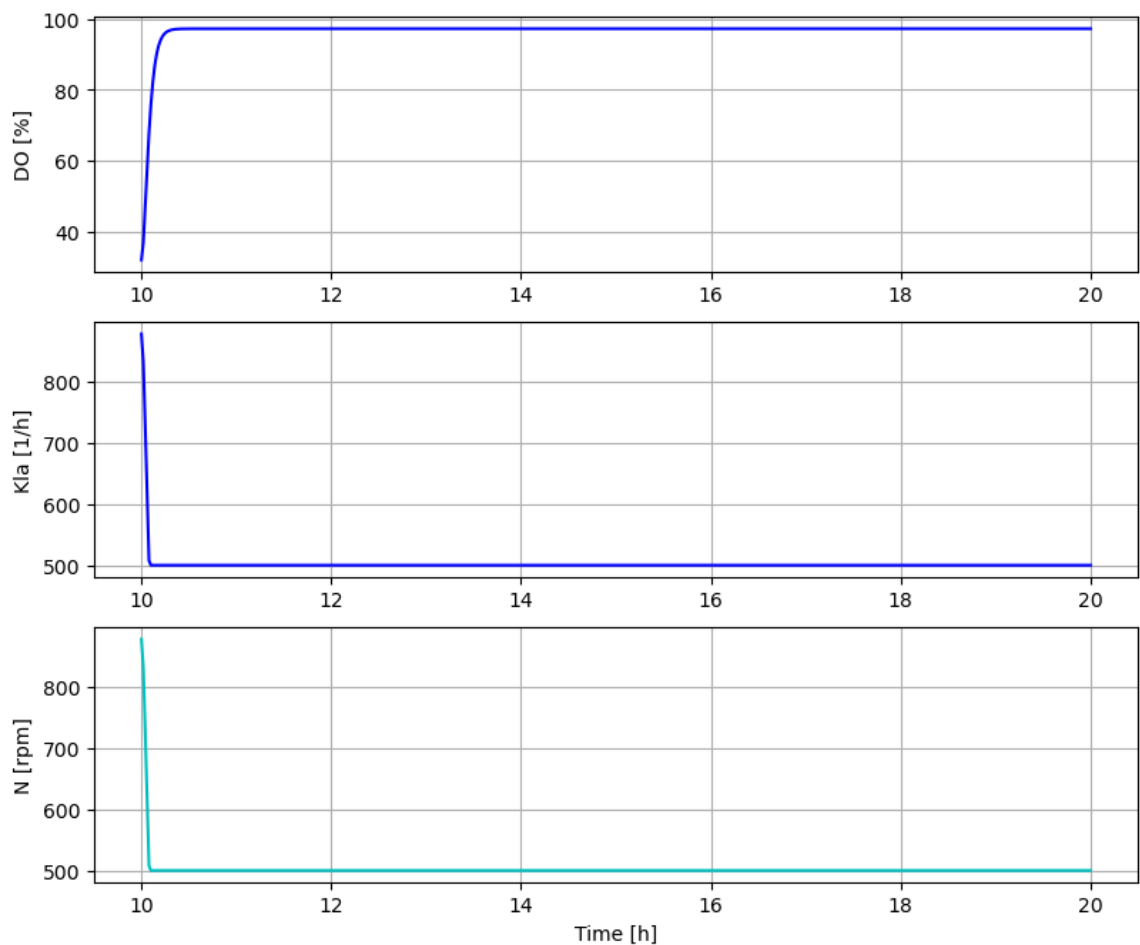


```
In [37]: # - study the variation of Kla together with DO and N during cultivation
plt.figure()
ax1 = plt.subplot(3,1,1); ax2 = plt.subplot(3,1,2); ax3 = plt.subplot(3,1,3)
ax1.set_ylabel('DO [%]'); ax1.grid()
ax2.set_ylabel('Kla [1/h]'); ax2.grid()
ax3.set_ylabel('N [rpm]'); ax3.grid()
ax3.set_xlabel('Time [h]')
```

```

setLines()
diagrams.clear()
diagrams.append("ax1.plot(sim_res['time'], sim_res['DOsensor.out'], color
diagrams.append("ax2.plot(sim_res['time'], sim_res['bioreactor.gas_liquid
diagrams.append("ax3.plot(sim_res['time'], sim_res['bioreactor.N'], color
show()

```



The relation is $KLa = \alpha_{O2} \cdot N$ and we see the value of the parameter should be around 1.0, and we check below

```

In [38]: disp('bioreactor.gas_liquid_transfer.alpha_O2')
alpha_O2 : 1.0

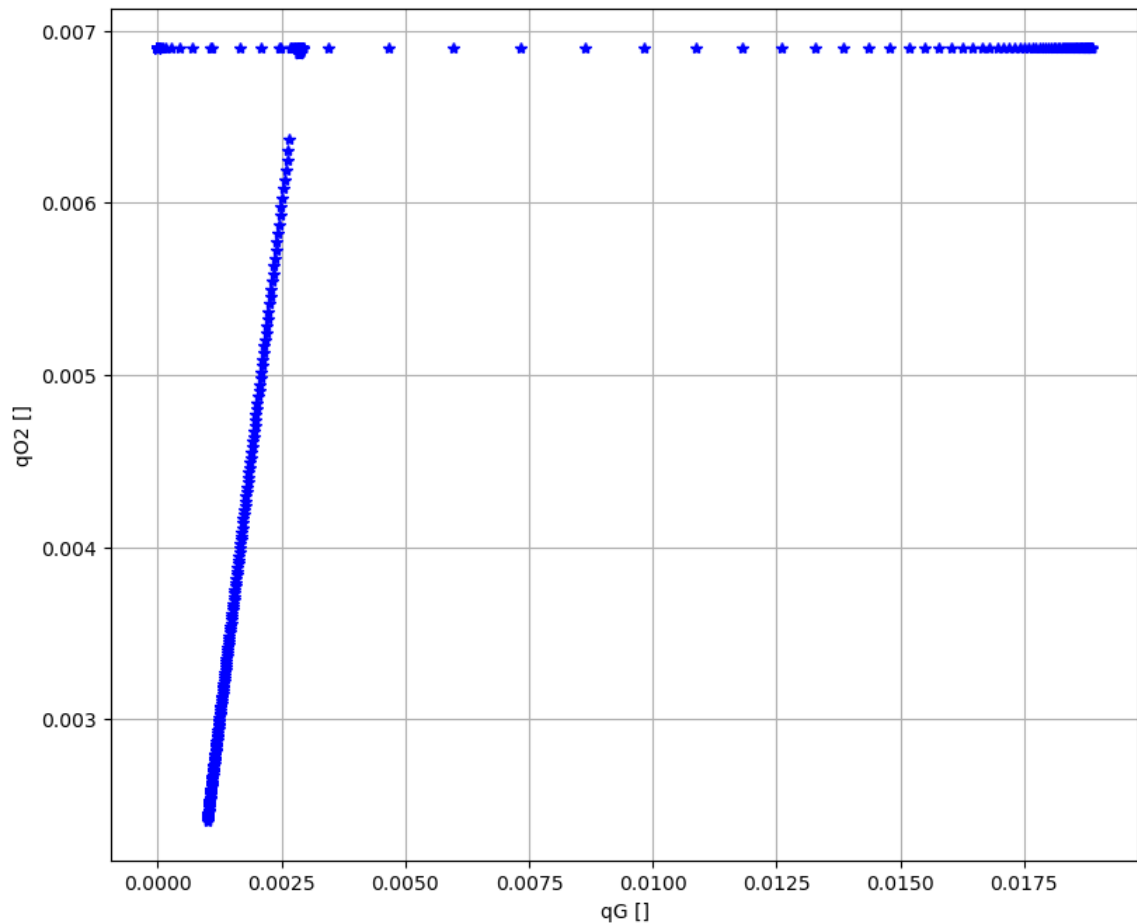
```

```

In [39]: # - study the relation qO2 vs qG(G)
plt.figure()
ax1 = plt.subplot(1,1,1)
ax1.set_ylabel('qO2 [ ]')
ax1.set_xlabel('qG [ ]')
ax1.grid()

setLines()
diagrams.clear()
diagrams.append("ax1.plot(sim_res['bioreactor.culture.qGm'], sim_res['bio
par(F_start=0.057, mu_feed=0.26)
simu(20)

```



During the cultivation we have a number of data points for q_G and q_{O_2} at the same time, during different conditions. What we see in the diagram is that q_{O_2} increase with q_G until q_G reach a level of just above 0.0025 and then q_{O_2} saturats for higher q_G . This what expect to see.

We also see that for lower q_G we have also q_{O_2} values at saturation level. This points correspond to a situation where ethanol is consumed with the remaining respiratory capacity. Glucose is consumed by priority.

Summary

- We have first seen an overview diagram of a typical yeast fedbatch cultivation where the feed started about an hour after the batch phase was finished. A new simulation was made where the feed started directly after detection of lack of substrate.
- We also took a look at the DO-control system and saw that we could decrease the control error by increasing the PI-controller gain. Stability of the control system remained.
- Then we tested variations in the feed dosage scheme and investigated the possibilities to increae the production.
- We also saw what happens if the feed dosage exceed the culture respiratory capacity and what to look for during the experimental work.
- Finally we saw some examples of how to improvise new diagrams.

References

[1] Sonnleitner, B and O. Käppeli "Growth of *Sacharomyces cerevisiae* is controlled by its limited respiratory capacity: formulation and verification of a hypothesis", Biotech. Bioeng., 1986.

[2] von Stockar, U., Gustafsson, L., Larsson, C., Marison, I., Tissot, P. and Gnaiger E. "Thermodynamic considerations in constructing energy balances for cellular growth", Biochimica et Biophysics Acta, vol 1183, p 221-240, 1993.

[3] Axelsson, J. P. "Experimental techniques and data analysis to determine baker's yeast ethanol dynamics", Anal. Chim. Acta, vol 213, p 151-163, 1988.

Appendix

```
In [40]: # List of components in the process setup and also a couple of other things
describe('parts')
```

```
['airFlow_setpoint', 'airtube', 'atmosphere', 'bioreactor', 'bioreactor.
culture', 'bioreactor.gas_liquid_transfer', 'compressor', 'D0_setpoint',
'dosagescheme', 'D0sensor', 'feedtank', 'N_high', 'N_low', 'PIreg', 'pump']
```

```
In [41]: describe('MSL')
```

```
MSL: 3.2.3 - used components: RealInput, RealOutput, LimPID-components
```

```
In [42]: system_info()
```

```
System information
-OS: Linux
-Python: 3.8.16
-Scipy: not installed in the notebook
-PyFMI: 2.9.8
-FMU by: OpenModelica Compiler OpenModelica 1.21.0~dev-266-g38c7170
-FMI: 2.0
-Type: FMUModelME2
-Name: BPL_YEAST_AIR.Fedbatch_D0control
-Generated: 2023-02-22T13:36:45Z
-MSL: 3.2.3
-Description: Bioprocess Library version 2.1.1-beta
-Interaction: FMU-explore version 0.9.7-beta
```

```
In [ ]:
```