

Supplementary material

‘A’ and ‘A+’ screw configurations with the applied screw elements are illustrated in Figures S1 and S2, respectively.

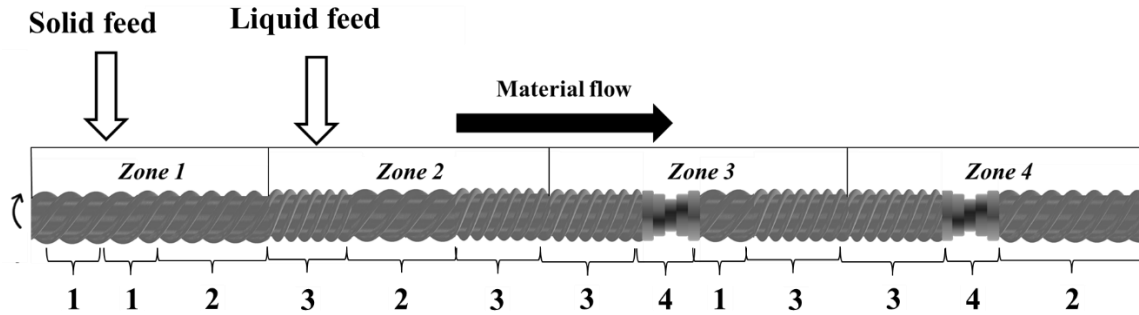


Figure S1: The ‘A’ screw configuration with the applied screw elements:
 (1) conveying element (22 mm length, 22 mm pitch);
 (2) conveying element (48 mm length, 16 mm pitch);
 (3) conveying element (30 mm length, 10 mm pitch);
 (4) five kneading elements (4 mm length each; offsets: 0°, 45°, 90°, 135°, 0°);

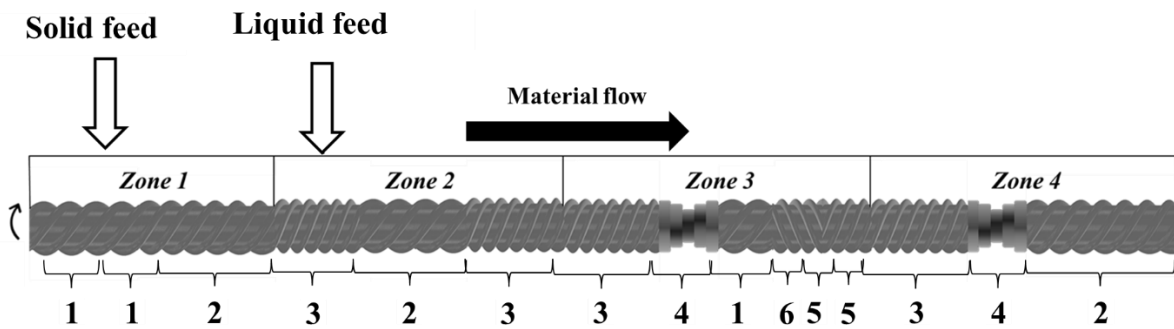


Figure S2: The ‘A+’ screw configuration with the applied screw elements:
 (1) conveying element (22 mm length, 22 mm pitch);
 (2) conveying element (48 mm length, 16 mm pitch);
 (3) conveying element (30 mm length, 10 mm pitch);
 (4) five kneading elements (4 mm length each; offsets: 0°, 45°, 90°, 135°, 0°);
 (5) reverse conveying element (10 mm length, 10 mm pitch);
 (6) conveying element (10 mm length, 10 mm pitch).

The experiments performed during the development and application of MLP and NARX models are summarized in Table S1.

Table S1: The applied process parameters of the experiments used for the development and application of MLP and NARX models.

Experiment number	Setting	Powder mass flow (kg/h)	L/S (-)	Temperature of the drying air (°C)*	Flow rate of the drying air (L/min)
P.1	1	1	0.11	30	90

Experiment number	Setting	Powder mass flow (kg/h)	L/S (-)	Temperature of the drying air (°C)*	Flow rate of the drying air (L/min)
	2	1	0.11	30	120
	3	1	0.11	30	60
	4	1	0.08	30	60
	5	1	0.08	30	120
	6	1	0.14	30	120
	7	1	0.14	30	60
	1	2	0.08	30	120
	2	2	0.14	30	60
	3	1	0.14	30	120
	4	1	0.08	30	60
	5	2	0.11	40	90
	6	1	0.14	50	120
P.2	7	2	0.08	50	120
	8	1	0.08	50	60
	9	2	0.14	50	60
	10	1	0.14	90	120
	11	1	0.08	90	60
	12	2	0.08	90	120
	13	2	0.14	90	60
	14	1	0.14	20	60
	1	2	0.08	30	60
	2	1	0.08	30	120
	3	1	0.14	30	120
	4	1	0.08	30	60
P.3	5	2	0.14	30	120
	6	1	0.14	30	60
	7	2	0.14	30	60
	8	2	0.08	30	120
	9	1	0.14	50	120
P.4	1	2	0.14	90	120

Experiment number	Setting	Powder mass flow (kg/h)	L/S (-)	Temperature of the drying air (°C)*	Flow rate of the drying air (L/min)
	2	2	0.14	50	120
	3	1	0.14	30	120
	4	2	0.14	30	60
	5	1	0.14	50	120
	6	1	0.14	90	60
P.5	1	2	0.14	30	120
	2	2	0.14	90	60
	3	2	0.14	50	60
	4	2	0.14	30	60
	5	1	0.14	50	60
	6	1	0.14	90	60
P.6	1	1	0.14	30	60
	2	1	0.14	50	120
	3	1	0.14	90	120
	4	1	0.14	30	120
	5	1	0.14	30	60

**referring to the temperature of Zones 1-3 during Experiment 1-3, while meaning the temperature of all zones during Experiment 4-6.*

The operation parameters collected from each unit with the SIPAT software are summarized in Table S2.

Table S2: The operation parameters registered by the SIPAT Simatic software.

Operation unit	Registered parameter
Gravimetric feeder	Feed rate (kg/h)
Granulation liquid feeding (balance)	The mass of the remaining granulation liquid (g)
Twin-screw granulator	Screw speed (rpm)
	Torque
	Temperature of zone 1 (°C)
	Temperature of zone 2 (°C)
	Temperature of zone 3 (°C)
	Temperature of zone 4 (°C)
Horizontal fluidized bed dryer	Vibratory intensity (Hz)

Operation unit	Registered parameter
	Temperature of zone 1 (°C)
	Temperature of zone 2 (°C)
	Temperature of zone 3 (°C)
	Temperature of zone 4 (°C)
	Flow rate of zone 1 (L/min)
	Flow rate of zone 2 (L/min)
	Flow rate of zone 3 (L/min)
	Flow rate of zone 4 (L/min)
Continuous mill	Oscillation speed (1/min)

The MLP model was trained using data collected during previous experiments. The utilized data is summarized in Table S3.

Table S3: Applied process parameters of the experiments that were used to train the MLP model.

Average drying airflow rate in Zone 1-4 (l/min)	Average drying temperature in Zone 1-3 (°C)	Powder mass flow (kg/h)	L/S (-)	Screw speed (rpm)	Average drying temperature in Zone 4 (°C)	Granulation temperature in Zone 4 (°C)	Granulation temperature in Zone 3 (°C)	Granulation temperature in Zone 2 (°C)	Granulation temperature in Zone 1 (°C)	Mill type* (-)	Mill sieve size diameter (mm)	Moisture content (%)
30	60	3	0.1	600	28.97	25	25	25	25	1	800	5.139
30	60	3	0.1	600	28.97	25	25	25	25	1	800	5.429
30	60	3	0.12	600	28.97	25	25	25	25	1	800	5.664
30	60	3	0.14	600	28.97	25	25	25	25	1	800	7.147
30	60	2	0.1	400	28.97	25	25	25	25	1	800	4.319
30	60	2	0.14	400	28.97	25	25	25	25	1	800	5.893
30	60	2	0.16	400	28.97	25	25	25	25	1	800	7.996
30	60	2	0.08	400	28.97	25	25	25	25	1	800	2.744
30	60	2	0.06	400	28.97	25	25	25	25	1	800	1.737
30	60	2	0.14	400	28.97	25	25	25	25	1	800	5.569
30	60	1	0.12	100	28.97	25	25	25	25	1	800	2.73
30	50	2	0.12	200	28.97	25	25	25	25	1	800	7.24
30	50	3	0.12	600	28.97	25	25	25	25	1	800	6.17
90	110	3	0.12	600	37.2	25	25	25	25	1	800	1.56
37	60	1	0.12	200	28.85	25	25	25	25	1	800	0.71
25	40	2	0.12	200	27.13	25	25	25	25	1	800	6.557
30	60	2	0.12	200	28.97	25	25	25	25	1	800	6.001
50	80	2	0.12	200	29.6	25	25	25	25	1	800	3.823
80	80	2	0.12	200	35.02	25	25	25	25	1	800	2.001
80	100	2	0.12	200	35.02	25	25	25	25	1	800	1.09
100	100	2	0.12	200	37.89	25	25	25	25	1	800	1.092
100	120	2	0.12	200	37.89	25	25	25	25	1	800	0.677
120	120	2	0.12	200	37.89	25	25	25	25	1	800	0.782

Average drying airflow rate in Zone 1-4 (l/min)	Average drying temperature in Zone 1-3 (°C)	Powder mass flow (kg/h)	L/S (-)	Screw speed (rpm)	Average drying temperature in Zone 4 (°C)	Granulation temperature in Zone 4 (°C)	Granulation temperature in Zone 3 (°C)	Granulation temperature in Zone 2 (°C)	Granulation temperature in Zone 1 (°C)	Mill type* (-)	Mill sieve size diameter (mm)	Moisture content (%)
25	40	1	0.12	200	27.13	33	33	33	33	2	800	4.869
25	70	1	0.12	200	27.13	37	37	37	37	2	800	4.167
50	140	1	0.12	200	29.6	42	42	42	42	2	800	1.783
40	120	3	0.12	300	29.27	27	27	27	27	2	800	4.769
60	140	3	0.12	300	31.4	27	27	27	27	2	800	3.595
100	140	3	0.12	300	37.89	27	27	27	27	2	800	2.625
25	60	1	0.12	100	27.13	27	27	27	27	2	800	3.808
25	60	1	0.12	100	27.13	28	28	28	28	2	800	5.407
25	60	1	0.12	300	27.13	37	37	37	37	2	800	2.977
25	60	3	0.12	300	27.13	38	38	38	38	2	800	5.47
40	120	3	0.12	300	29.27	44	44	44	44	2	800	3.696
60	140	3	0.12	300	31.4	44	44	44	44	2	800	2.055
100	140	3	0.12	300	37.89	43	43	43	43	2	800	0.654
60	90	1.5	0.11	300	28.5	29	28	26	26	1	800	0.961
30	120	1	0.14	200	28.6	29	27	26	26	1	800	2.504
30	120	1	0.08	200	28.6	28	27	26	25	1	800	0.719
30	60	2	0.08	400	28.3	29	28	26	25	1	800	2.707
30	60	1	0.14	200	28.3	29	27	26	25	1	800	3.532
30	120	2	0.08	400	28.3	29	27	26	25	1	800	1.148
30	120	2	0.14	400	28.6	30	28	26	25	1	800	4.636
30	60	2	0.14	400	28.4	31	28	26	25	1	800	7.013
30	60	1	0.08	200	28.5	29	27	25	25	1	800	1.606
60	90	1.5	0.11	300	30.9	29	27	25	25	1	800	1.112
90	120	1	0.14	200	35.2	27	26	25	25	1	800	0.474
90	60	2	0.08	400	35.3	29	27	25	25	1	800	0.371
90	60	1	0.08	200	35.9	27	26	25	25	1	800	0
90	60	1	0.14	200	36.6	27	26	25	25	1	800	0.589
90	120	1	0.08	200	38.2	26	25	25	25	1	800	0
90	120	2	0.08	400	39.1	29	27	25	25	1	800	0.01
90	120	2	0.14	400	39.3	30	28	26	25	1	800	0.531
90	60	2	0.14	400	38	31	28	26	25	1	800	0.895
60	90	1.5	0.11	300	34.8	29	27	26	25	1	800	0.793
30	60	2	0.08	400	28.8	28	28	27	27	1	800	2.504
30	120	1	0.08	200	28.7	27	27	26	26	1	800	0.672
30	120	1	0.14	200	28.7	28	27	26	26	1	800	2.649
30	60	1	0.08	200	28.6	27	26	25	25	1	800	1.402
30	120	2	0.14	400	28.8	30	28	26	26	1	800	5.815
30	60	1	0.14	200	28.7	28	26	25	25	1	800	4.689
40	90	1.5	0.11	300	27.2	29	27	27	30	1	800	2
50	120	1	0.14	200	28.1	29	27	27	29	1	800	1.73
50	60	2	0.08	400	28.1	29	27	27	29	1	800	2.08
50	60	1	0.08	200	28.3	29	26	27	29	1	800	1.15
50	60	1	0.14	200	28.8	28	26	27	30	1	800	3.02

Average drying airflow rate in Zone 1-4 (l/min)	Average drying temperature in Zone 1-3 (°C)	Powder mass flow (kg/h)	L/S (-)	Screw speed (rpm)	Average drying temperature in Zone 4 (°C)	Granulation temperature in Zone 4 (°C)	Granulation temperature in Zone 3 (°C)	Granulation temperature in Zone 2 (°C)	Granulation temperature in Zone 1 (°C)	Mill type* (-)	Mill sieve size diameter (mm)	Moisture content (%)
50	120	1	0.08	200	29.6	27	26	27	30	1	800	0.75
50	120	2	0.08	400	30	28	27	27	30	1	800	0.72
50	120	2	0.14	400	30.2	31	28	27	30	1	800	2.82
50	60	2	0.14	400	29.9	31	28	27	30	1	800	4.55
40	90	1.5	0.11	300	29.9	30	28	27	30	1	800	1.81
30	60	2	0.08	400	28.8	28	26	27	31	1	800	2.3
30	120	1	0.08	200	28.9	26	25	27	31	1	800	0.96
30	120	1	0.14	200	28.8	27	26	27	31	1	800	2.24
30	60	1	0.08	200	28.6	27	25	27	31	1	800	1.65
30	120	2	0.14	400	28.7	31	28	26	25	1	800	3.21
30	60	1	0.14	200	28.5	29	27	26	25	1	800	3.46
30	60	2	0.14	400	28.4	31	28	26	25	1	800	5.49
30	120	2	0.08	400	28.6	30	28	26	26	1	800	1.65
40	90	1.5	0.11	300	28.8	30	28	26	25	1	800	1.88
50	120	1	0.08	200	29.9	28	26	25	25	1	800	1.09
50	120	2	0.14	400	30.3	31	28	26	25	1	800	2.91
50	60	2	0.14	400	30	32	29	26	26	1	800	4.41
50	120	1	0.14	200	30.6	30	28	26	25	1	800	1.57
50	120	2	0.08	400	30.8	30	28	26	26	1	800	1.03
50	60	1	0.08	200	30.5	28	27	25	25	1	800	1.06
50	60	2	0.08	400	30.5	29	27	26	26	1	800	1.36
50	60	1	0.14	200	30.6	28	27	25	25	1	800	1.86
40	90	1.5	0.11	300	30.6	29	27	26	26	1	800	1.77
30	120	1	0.14	200	29.7	28	27	25	25	1	800	2.09
30	120	1	0.08	200	29.7	27	26	25	25	1	800	1.23
30	60	2	0.08	400	29.5	28	27	25	25	1	800	2.24
30	60	1	0.14	200	29.4	28	27	25	25	1	800	2.42
30	120	2	0.08	400	29.5	29	27	25	26	1	800	1.83
30	120	2	0.14	400	29.4	31	29	26	26	1	800	2.49
30	60	2	0.14	400	29.1	31	29	27	26	1	800	5.21
30	60	1	0.08	200	29.1	30	28	26	26	1	800	1.63
40	90	1.5	0.11	300	27.5	31	28	25	24	1	800	2.05
70	120	1	0.14	200	30.2	27	26	24	24	1	800	0.76
70	60	2	0.08	400	30.2	26	25	24	24	1	800	0.99
70	60	1	0.08	200	30.9	24	24	23	24	1	800	0.56
70	60	1	0.14	200	31.1	24	24	23	24	1	800	0.72
70	120	1	0.08	200	32.4	25	24	23	24	1	800	0.31
70	120	2	0.08	400	32.8	25	24	24	24	1	800	0.44
70	120	2	0.14	400	33.1	28	27	25	24	1	800	1.28
70	60	2	0.14	400	32.5	30	28	25	24	1	800	3.63
40	90	1.5	0.11	300	30.4	29	29	26	25	1	800	1.75
40	90	1.5	0.11	300	29.9	29	29	27	25	1	800	1.74

Table S4 summarizes the training-control hyperparameters used during the training of the MLP model with Bayesian regularization.

Table S4: Training-control hyperparameters used during MLP model training with Bayesian regularization.

Parameter	Description	Value
net.trainParam.epochs	Maximum number training epochs	1000
net.trainParam.goal	Performance goal (MSE target)	0
net.trainParam.mu	Marquardt adjustment parameter	0.005
net.trainParam.mu_dec	Decrease factor for mu if performance improves	0.1
net.trainParam.mu_inc	Increase factor for mu if performance worsenes	10
net.trainParam.mu_max	Maximum value for mu.	1e10
net.trainParam.max_fail	Maximum consecutive validation failures before stopping	0
net.trainParam.min_grad	Minimum performance gradient to continue training	1e ⁻⁷
net.trainParam.time	Maximum time to train in seconds.	inf.

The applied filters to the input data of the NARX and the moisture content determined by the PLS model are summarized in Table S5.

Table S5: Window sizes used for smoothing parameters with a moving average

Registered parameter	Window size
Solid feed rate	120 s
Liquid feed rate	60 s
L/S ratio	120 s
Drying temperature (average of Zone 1-3)	120 s
Flow rate of the drying air (average of Zone 1-4)	60 s
Moisture content (detected by the PLS model)	180 s