Appendices (A-C)

Title: **A Unified Benchmark for Security and Reliability Assessment of the Integrated Chemical Plant, Natural Gas and Power Transmission Networks**

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Appendix A. Data for the gas pipeline and geographical coordinates of the syngas plant, natural gas, and power transmission networks.

The pipeline data as well as the geographical coordinates of the Syngas plant, natural gas, and power transmission networks are given in Table A.1 to Table A.5.

Starting Node	Ending Node	Length [Km]	Diameter [m]
1	2	100	0.9144
2	3	30	0.6350
3	4	5	0.6350
4	5	15	0.6350
5	6	10	0.6350
6	7	5	0.6350
7	8	10	0.6350
8	9	5	0.9144
9	10	60	0.9144
10	11	5	0.6350
11	12	8	0.6350
11	13	6	0.6350
10	14	80	0.9144
14	15	10	0.9144
15	16	20	0.9144
16	17	3	0.6350
17	18	6	0.6350
16	19	5	0.6350
15	20	40	0.9144
20	21	5	0.9144
21	22	20	0.9144
22	23	5	0.9144
23	24	16	0.9144

Node Number	Type	Latitude	Longitude
1	supply	32.73863	-114.63904
2	Node	32.99842	-115.50248
3	Node	32.91879	-115.76985
4	Node	32.78977	-115.85446
5	Node	32.73448	-116.0316
6	SynGas Demand	32.63406	-116.20342
7	Node	32.7819	-116.13369
8	Power Demand	32.81886	-116.32434
9	Node	33.06292	-115.39132
10	Node	33.54045	-114.9868
11	Node	33.52901	-115.16741
12	Demand	33.68336	-115.17709
13	Power Demand	33.50618	-115.3295
14	Node	33.65556	-114.2273
15	Node	33.67138	-113.99405
16	Node	33.63961	-113.74963
17	Node	33.59129	-113.55726
18	Demand	33.57985	-113.36486
19	Power Demand	33.73234	-113.67656
20	Node	33.86509	-113.97678
21	Node	33.97907	-114.07031
22	Node	34.02234	-114.22682
23	Node	34.10874	-114.13616

22	25	8	0.6350

Table A1.
The natural gas pipeline data [1] .

24	Power Demand	34.21138	-114.13185
25	Demand	34.14052	-114.28999

Table A3.
The natural gas topology data.

Bus ID	Latitude	Longitude
1	33.396	-113.836
2	33.358	-113.826
3	33.537	-114.670
4	33.812	-113.825
5	33.659	-113.999
6	33.738	-114.182
7	33.732	-113.677
8	34.459	-113.762
9	33.920	-114.308
10	33.913	-114.293
11	33.904	-114.301
12	33.911	-114.3134
13	34.211	-114.132
14	33.777	-114.820
15	33.506	-115.329
16	33.661	-115.321
17	33.575	-115.641
18	33.544	-115.801
19	33.869	-115.369
20	34.244	-115.262
21	33.527	-116.071
22	32.818	-116.324
23	34.382	-115.069
24	33.543	-114.656

Table A.2
Power network topology data.

Latitude	Longitude
32.63406	-116.20342

Table A.4
SynGas plant topology data.

Node number	ρ	φ
1	1.48473	0.031129
2	1.448602	0.031129
3	1.41155	0.031129
4	1.373498	0.031129
5	1.334362	0.031129
6	1.294042	0.031129
7	1.252426	0.031129
8	1.209378	0.031129
9	1.16474	0.031129
10	1.118321	0.031129

11	1.116204	0.005481
12	1.114084	0.005481
13	1.111959	0.005481
14	1.422476	0.005481
15	1.421228	0.005481
16	1.41998	0.005481
17	1.419563	0.00274
18	1.419772	0.00274
19	1.419355	0.00274
20	1.463949	0.025649
21	1.439167	0.025649
22	1.413951	0.025649
23	1.388276	0.025649
24	1.362118	0.025649
25	1.335448	0.025649
26	1.308234	0.025649
27	1.306561	0.007454
28	1.306546	0.000548
29	1.304836	0.006905
30	1.294322	0.018195
31	1.280259	0.018195
32	1.26604	0.018195
33	1.251659	0.018195
34	1.237111	0.018195
35	1.22239	0.018195
36	1.207489	0.018195
37	1.192403	0.018195
38	1.478308	0.018195
39	1.472212	0.012824
40	1.46609	0.012824
41	1.466086	0.000548
42	1.466076	0.000548
43	1.462038	0.012276
44	1.47724	0.005371
45	1.476172	0.005371
46	1.475103	0.005371
47	1.474034	0.005371
48	1.53248	0.005371
49	1.531451	0.005371
50	1.53042	0.005371
51	1.530005	0.004823
52	1.52934	0.004823
53	1.528674	0.004823

54	1.530408	0.000548

Table A.5

The initial condition data of gas network.

Appendix B. Data for the power transmission network in the nominal condition

Table B.6 to Table B.9 provide the base case data for the power transmission network in its nominal operating condition of the integrated system.

Bus_I	Bus_Type	P_d	Q_d	G_s	B_s	area	V_m	V_a	Base KV	zone	V_{max}	V_{min}
1	2	93.2256	18.9904	0	0	1	1	0	138	1	1.05	0.95
2	2	83.7304	17.264	0	0	1	1	0	138	1	1.05	0.95
3	1	155.376	31.9384	0	0	1	1	0	138	1	1.05	0.95
4	1	63.8768	12.948	0	0	1	1	0	138	1	1.05	0.95
5	1	61.2872	12.0848	0	0	1	1	0	138	1	1.05	0.95
6	1	68	14	0	-100	2	1	0	138	1	1.05	0.95
7	2	107.9	21.58	0	0	2	1	0	138	1	1.05	0.95
8	1	147.6072	30.212	0	0	2	1	0	138	1	1.05	0.95
9	1	87.5	18	0	0	1	1	0	138	1	1.05	0.95
10	1	97.5	20	0	0	2	1	0	138	1	1.05	0.95
11	1	0	0	0	0	3	1	0	230	1	1.05	0.95
12	1	0	0	0	0	3	1	0	230	1	1.05	0.95
13	3	228.748	46.6128	0	0	3	1	0	230	1	1.05	0.95
14	2	97	19.5	0	0	3	1	0	230	1	1.05	0.95
15	2	158.5	32	0	0	4	1	0	230	1	1.05	0.95
16	2	86.32	17.264	0	0	4	1	0	230	1	1.05	0.95
17	1	0	0	0	0	4	1	0	230	1	1.05	0.95
18	2	166.5	34	0	0	4	1	0	230	1	1.05	0.95
19	1	90.5	18.5	0	0	3	1	0	230	1	1.05	0.95
20	1	64	13	0	0	3	1	0	230	1	1.05	0.95
21	2	0	0	0	0	4	1	0	230	1	1.05	0.95
22	2	0	0	0	0	4	1	0	230	1	1.05	0.95
23	2	0	0	0	0	3	1	0	230	1	1.05	0.95
24	1	0	0	0	0	4	1	0	230	1	1.05	0.95

Table B.6
Bus data of the power transmission network in the base case [2].

Bus number	Type of load A, B, Const	Bus load % of load system	Load $[MW]$	If peak load 25 %higher $[MW]$
1	B	4.85	86.4	108
2	A	4.35	77.6	97
3	A	8.08	144	180
4	A	3.32	59.2	74
5	A	3.19	56.8	71

6	Const	3.81	68	85
7	B	5.61	100	125
8	B	7.68	136.8	171
9	Const	4.91	87.5	109.375
10	Const	5.47	97.5	121.875
13	A	11.89	212	265
14	Const	5.44	97	121.25
15	Const	8.89	158.5	198.125
16	B	4.49	80	100
18	Const	9.34	166.5	208.125
19	Const	5.08	90.5	113.125
20	Const	3.59	64	80
		Total 100		

Table B.7
Bus load data of the power transmission network in the base case [2].

Bus	P_g	Q_g	Q_{max}	Q_{min}	V_g	mBase	Status	P_{max}	P_{min}
1	10	0	8	0	1.035	100	1	16	8
1	10	0	8	0	1.035	100	1	16	8
1	60.8	0	24	-12.5	1.035	100	1	60.8	7.6
1	60.8	0	24	-12.5	1.035	100	1	60.8	7.6
2	12	0	8	0	1.035	100	1	16	8
2	12	0	8	0	1.035	100	1	16	8
2	60.8	0	24	-12.5	1.035	100	1	60.8	7.6
2	60.8	0	24	-12.5	1.035	100	1	60.8	7.6
7	60	0	48	0	1.025	100	1	80	8.333333
7	60	0	48	0	1.025	100	1	80	8.333333
7	60	0	48	0	1.025	100	1	80	8.333333
13	57.6	0	64	0	1.02	100	1	157.6	23
13	57.6	0	64	0	1.02	100	1	157.6	23
13	57.6	0	64	0	1.02	100	1	157.6	23
14	0	35.3	160	-50	0.98	100	1	0	0
15	9.6	0	4.8	0	1.014	100	1	9.6	0.48
15	9.6	0	4.8	0	1.014	100	1	9.6	0.48
15	9.6	0	4.8	0	1.014	100	1	9.6	0.48
15	9.6	0	4.8	0	1.014	100	1	9.6	0.48
15	9.6	0	4.8	0	1.014	100	1	9.6	0.48
15	124	0	64	-50	1.014	100	1	124	54.3
16	124	0	64	-50	1.017	100	1	124	54.3
18	320	0	160	-50	1.05	100	1	320	100
21	320	0	160	-50	1.05	100	1	320	100
22	40	0	12.8	-1.66667	1.05	100	1	40	1.666667
22	40	0	12.8	-1.66667	1.05	100	1	40	1.666667
22	40	0	12.8	-1.66667	1.05	100	1	40	1.666667
22	40	0	12.8	-1.66667	1.05	100	1	40	1.666667
22	40	0	12.8	-1.66667	1.05	100	1	40	1.666667
22	40	0	12.8	-1.66667	1.05	100	1	40	1.666667
23	124	0	64	-25	1.05	100	1	124	27.15

23	124	0	64	-25	1.05	100	1	124	27.15
23	280	0	120	-25	1.05	100	1	280	140

Table B.8
Generator data of the power transmission network in the base case [2].

F_Bus	T_Bus	r	X	b	$Rate\_A$	$Rate\_B$	$Rate\_C$	ratio	angle	Status	angmin	angmax
1	2	0.0026	0.0139	0.4611	140	250	200	0	0	1	-360	360
1	3	0.0546	0.2112	0.0572	140	208	220	0	0	1	-360	360
1	5	0.0218	0.0845	0.0229	140	208	220	0	0	1	-360	360
2	4	0.0328	0.1267	0.0343	140	208	220	0	0	1	-360	360
2	6	0.0497	0.192	0.052	140	208	220	0	0	1	-360	360
3	9	0.0308	0.119	0.0322	140	208	220	0	0	1	-360	360
3	24	0.0023	0.0839	0	320	510	600	1.03	0	1	-360	360
4	9	0.0268	0.1037	0.0281	140	208	220	0	0	1	-360	360
5	10	0.0228	0.0883	0.0239	140	208	220	0	0	1	-360	360
6	10	0.0139	0.0605	2.459	140	193	200	0	0	1	-360	360
7	8	0.0159	0.0614	0.0166	140	208	220	0	0	1	-360	360
8	9	0.0427	0.1651	0.0447	140	208	220	0	0	1	-360	360
8	10	0.0427	0.1651	0.0447	140	208	220	0	0	1	-360	360
9	11	0.0023	0.0839	0	320	510	600	1.03	0	1	-360	360
9	12	0.0023	0.0839	0	320	510	600	1.03	0	1	-360	360
10	11	0.0023	0.0839	0	320	510	600	1.02	0	1	-360	360
10	12	0.0023	0.0839	0	320	510	600	1.02	0	1	-360	360
11	13	0.0061	0.0476	0.0999	400	600	625	0	0	1	-360	360
11	14	0.0054	0.0418	0.0879	400	625	625	0	0	1	-360	360
12	13	0.0061	0.0476	0.0999	400	625	625	0	0	1	-360	360
12	23	0.0124	0.0966	0.203	400	625	625	0	0	1	-360	360
13	23	0.0111	0.0865	0.1818	400	625	625	0	0	1	-360	360
14	16	0.005	0.0389	0.0818	400	625	625	0	0	1	-360	360
15	16	0.0022	0.0173	0.0364	400	600	625	0	0	1	-360	360
15	21	0.0063	0.049	0.103	400	600	625	0	0	1	-360	360
15	21	0.0063	0.049	0.103	400	600	625	0	0	1	-360	360
15	24	0.0067	0.0519	0.1091	400	600	625	0	0	1	-360	360
16	17	0.0033	0.0259	0.0545	400	600	625	0	0	1	-360	360
16	19	0.003	0.0231	0.0485	400	600	625	0	0	1	-360	360
17	18	0.0018	0.0144	0.0303	400	600	625	0	0	1	-360	360
17	22	0.0135	0.1053	0.2212	400	600	625	0	0	1	-360	360
18	21	0.0033	0.0259	0.0545	400	600	625	0	0	1	-360	360
18	21	0.0033	0.0259	0.0545	400	600	625	0	0	1	-360	360
19	20	0.0051	0.0396	0.0833	400	600	625	0	0	1	-360	360
19	20	0.0051	0.0396	0.0833	400	600	625	0	0	1	-360	360
20	23	0.0028	0.0216	0.0455	400	600	625	0	0	1	-360	360
20	23	0.0028	0.0216	0.0455	400	600	625	0	0	1	-360	360
21	22	0.0087	0.0678	0.1424	400	600	625	0	0	1	-360	360

Table B.9

Branch data of the power transmission network in the base case [2].

Appendix C. Correlations and Parameters for the SynGas plant

The equations and correlations for calculating the physical properties, reaction rates, constants, and parameters are given by the equations (C.1)-(C.28) and Table C.10 [3].

$$u_{s,0} = \frac{F_{total,0}.R.T_0}{\Omega p_0} \tag{C.1}$$

$$u_s = u_{s,0}\frac{F_{total}.p_0.T}{F_{total,0}.p.T_0} \tag{C.2}$$

$$\varepsilon_B = \frac{0.9198}{(d_{tube}/d_{p,i})^2} + 0.3414 \tag{C.3}$$

$$\rho_b = \rho_s(1-\varepsilon_B) \tag{C.4}$$

$$D_{m,j} = \frac{1}{\sum_{j=1,j\neq i}^{n}\frac{y_j}{D_{m,ij}}} \tag{C.5}$$

$$\frac{(D.p)_H}{(D.p)} = function\ (T_R, p_R) \tag{C.6}$$

$$\frac{1}{D_{eff,j}} = \frac{\varepsilon}{T}\left(\frac{1}{D_{m,j}} + \frac{1}{D_{k,j}}\right) \tag{C.7}$$

$$D_{ax} = a.D_m + \frac{b.u_s.d_{p,i}/\varepsilon_B}{1+\frac{c.D_m}{u_s.d_{p,i}/\varepsilon_B}} \tag{C.8}$$

$$\lambda_{gm} = \sum_{i=1}^{n}\frac{y_i\lambda_{g,i}}{\sum_{j=1}^{n} y_j A_{ij}} \tag{C.9}$$

$$A_{ij} = \frac{[1+(\frac{\lambda_{tr,i}}{\lambda_{tr,j}})^{0.5}(\frac{MW_i}{MW_j})^{0.25}}{[8(1+\frac{MW_i}{MW_j})]^{0.5}} \tag{C.10}$$

$$\frac{\lambda_{tr,i}}{\lambda_{tr,j}} = \frac{\Gamma_j[\exp\left(0.00464T_{R,i}\right) - \exp(-0.2412T_{R,i})}{\Gamma_i[\exp\left(0.0464T_{R,i}\right) - \exp(-0.2412T_{R,i})} \tag{C.11}$$

$$\Gamma = 210(\frac{T_C MW^3}{P_C^4} \tag{C.12}$$

$$\frac{\lambda_{ax}}{\lambda_{gm}} = \frac{\lambda_{ax}^0}{\lambda_{gm}} + \delta N_{pr}N_{Re} \quad \delta = 0.75 \tag{C.13}$$

$$\frac{\lambda_{ax}^0}{\lambda_{gm}} = \varepsilon_B + \frac{1-\varepsilon_B}{0.139\varepsilon_B - 0.0339 + \frac{2\lambda_{gm}}{3\lambda_s}} \tag{C.14}$$

$$\frac{1}{U} = \frac{1}{a_W} + \frac{d_{tube,o}}{6\lambda_{er}}(\frac{Bi+3}{Bi+4}) \tag{C.15}$$

$$Bi = \frac{a_W d_{tube,o}}{2\lambda_{er}} \tag{C.16}$$

$$\lambda_{er} = \lambda_{er}^0 + 0.111\lambda_g \frac{N_{Re}N_{Pr}^{1/3}}{1+46(d_{p,i}/d_{tube,o})^2} \tag{C.17}$$

$$\lambda_{er}^0 = \varepsilon_B\left(\lambda_g + 0.95a_{ru}d_{p,i}\right) + \frac{0.95(1-\varepsilon)}{2/(3\lambda_s) + 1/(10\lambda_g + a_{rs}d_{p,i})} \tag{C.18}$$

$$a_{ru} = \frac{0.8171(T/100)^3}{1+\varepsilon_B/2(1-\varepsilon_B)(1-e_m)/e_m} \tag{C.19}$$

$$a_{rs} = 0.8171\frac{e_m}{2-e_m}(T/100)^3 \tag{C.20}$$

$$a_W = (1-1.5(\frac{d_{tube,i}}{d_{p,i}})^{-1.5})\frac{\lambda_g}{d_{p,i}}N_{Re}^{0.59}N_{pr}^{1/3} \tag{C.21}$$

$$r_1 = \frac{k_1}{p_{H_2}^{2.5}}\frac{p_{CH_4}p_{H_2o} - p_{H_2}^3 p_{CO}/K_1}{DEN^2} \tag{C.22}$$

$$r_2 = \frac{k_2}{P_{H_2}}\frac{p_{CO}p_{H_2o} - P_{H_2}p_{CO_2}/K_2}{DEN^2} \tag{C.23}$$

$$r_3 = \frac{k_3}{P_{H_2}^{3.5}}\frac{p_{CH_4}p_{H_2o}^2 - p_{H_2}^4 p_{CO_2}/K_3}{DEN^2} \tag{C.24}$$

$$DEN = 1 + K_{CO}P_{CO} + K_{H_2}P_{H_2} + K_{CH_4}p_{CH_4} + \frac{K_{H_2o}p_{H_2o}}{p_{H_2}} \tag{C.25}$$

$$k_i = A(k_i).\exp[-E_i/(RT)],\ \ for\ i = 1,\dots,3 \tag{C.26}$$

$$K_i = A(K_i).\exp[-\Delta H_i/(RT)],\ \ for\ i = 1,\dots,3 \tag{C.27}$$

$$K_j = A\left(K_j\right).\exp[-\Delta H_j/(RT)],\ \ for\ j = CH_4, H_2O, CO, H_2 \tag{C.28}$$

Activation energies (E), Heat of reactions $\Delta H_{1,2,3}$ and adsorption enthalpies $\Delta H_{component} [KJ/mol]$									
E_1	E_2	E_3	ΔH_1	ΔH_2	ΔH_3	ΔH_{CO}	ΔH_{H_2}	ΔH_{CH_4}	ΔH_{H_2O}

240.1 67.13 243.9 206.1 -41.15 164.9 -70.65 -82.90 -
38.28 88.68

$A(k_1)[kmol\ bar^{0.5} kg^{-1} hr^{-1}]$ $A(k_2)[kmol\ bar^{0.5} kg^{-1} hr^{-1}]$ $A(k_3)[kmol\ bar^{0.5} kg^{-1} hr^{-1}]$
$A(K_1)[bar^2]$ $A(K_2)[bar]$ $A(K_3)[bar^2]$

4.225×10^{15} 1.955×10^{6} 1.02×10^{15}

4.707×10^{12} 1.142×10^{-2} 5.375×10^{10}

$A(K_{CO})[bar^{-1}]$ $A\left(K_{H_2}\right)$ $A\left(K_{CH_4}\right)[bar^{-1}]$ $A\left(K_{H_2o}\right)[bar^{-1}]$

8.23×10^{-5} 6.12×10^{-9} 6.65×10^{-4} 1.77×10^{5}

Table C.10
The kinetic data required for the reaction rates of the steam methane reforming process [3].

References

[1] B. Zhao, A. Zlotnik, A. J. Conejo, R. Sioshansi, and A. M. Rudkevich, "Shadow price-based co-ordination of natural gas and electric power systems," *IEEE Transactions on Power Systems*, vol. 34, no. 3, pp. 1942-1954, 2018.

[2] A. Zlotnik, L. Roald, S. Backhaus, M. Chertkov, and G. Andersson, "Coordinated scheduling for interdependent electric power and natural gas infrastructures," *IEEE Transactions on Power Systems*, vol. 32, no. 1, pp. 600-610, 2016.

[3] G. Pantoleontos, E. S. Kikkinides, and M. C. Georgiadis, "A heterogeneous dynamic model for the simulation and optimisation of the steam methane reforming reactor," *International Journal of Hydrogen Energy*, vol. 37, no. 21, pp. 16346-16358, 2012.