Full Furnace Simulations and Optimization with COILSIM1D

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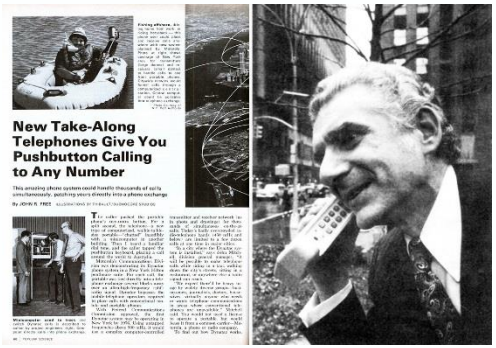
Change is inevitable

1977



2016

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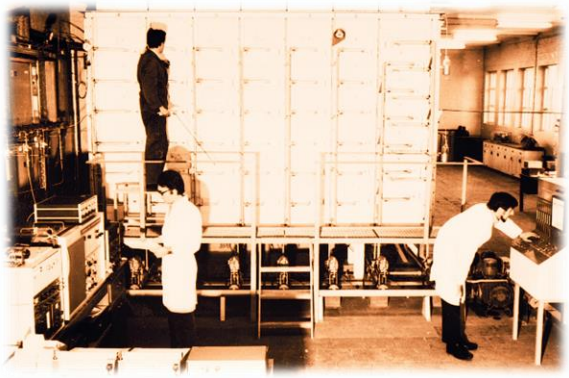
LCT's steam cracking timeline



Pilot plant starts operation

First commercial license sold

Implementation of GCxGC

Pilot plant revamped

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COILSIM3D, continuous expansion of kinetic network, …

1974 1976 1978 2001 2004 2006 2008 2010 2012 2015 2016

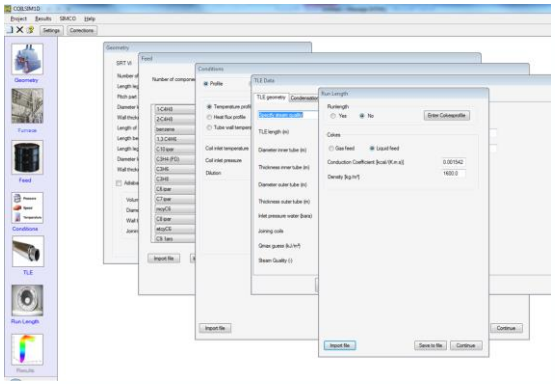
First simulations of steam cracking

First kinetics of coke formation

Large expansion of kinetic network

TLE model

COILSIM1D's **GUI** implementation



Kinetic expansion; Firebox and convection models

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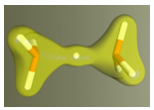
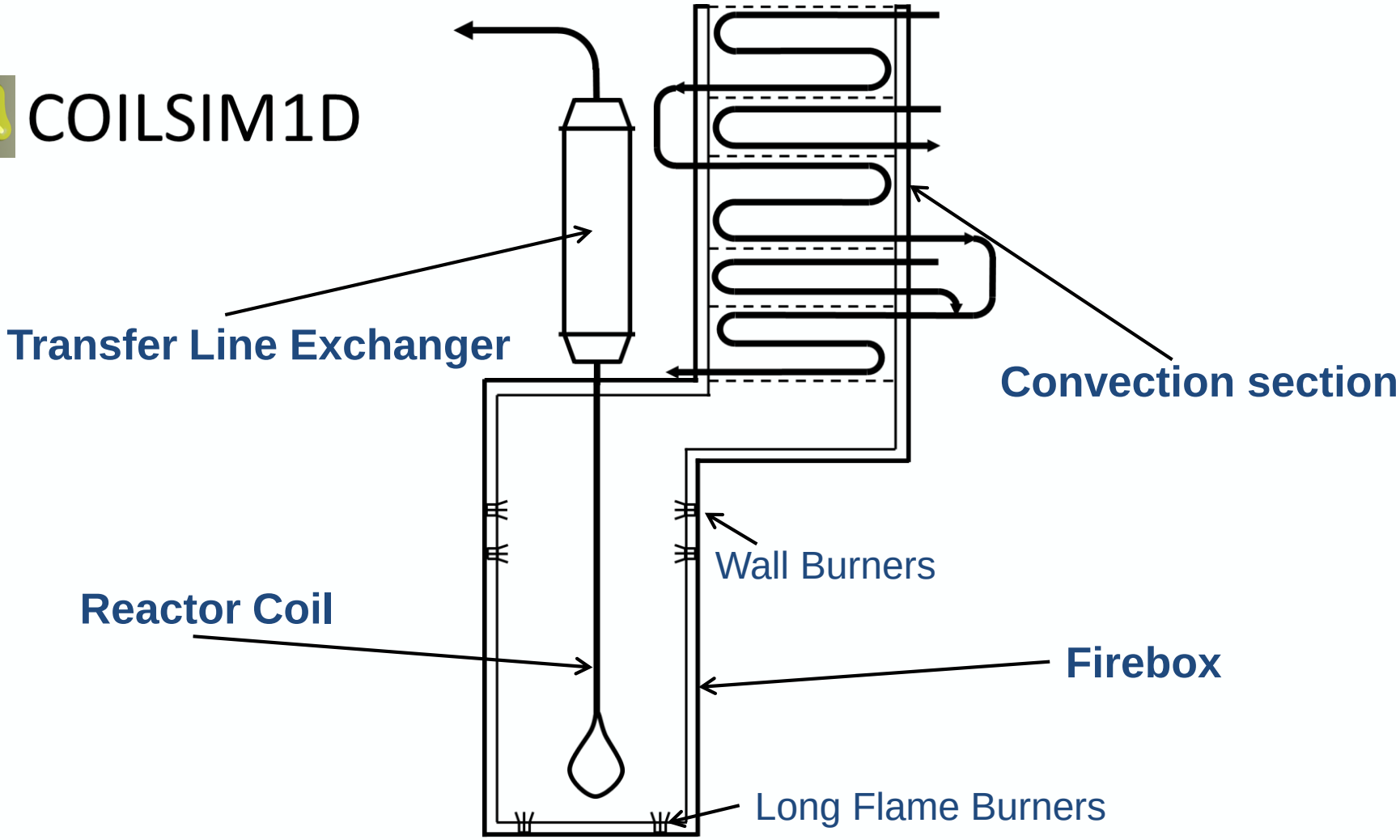
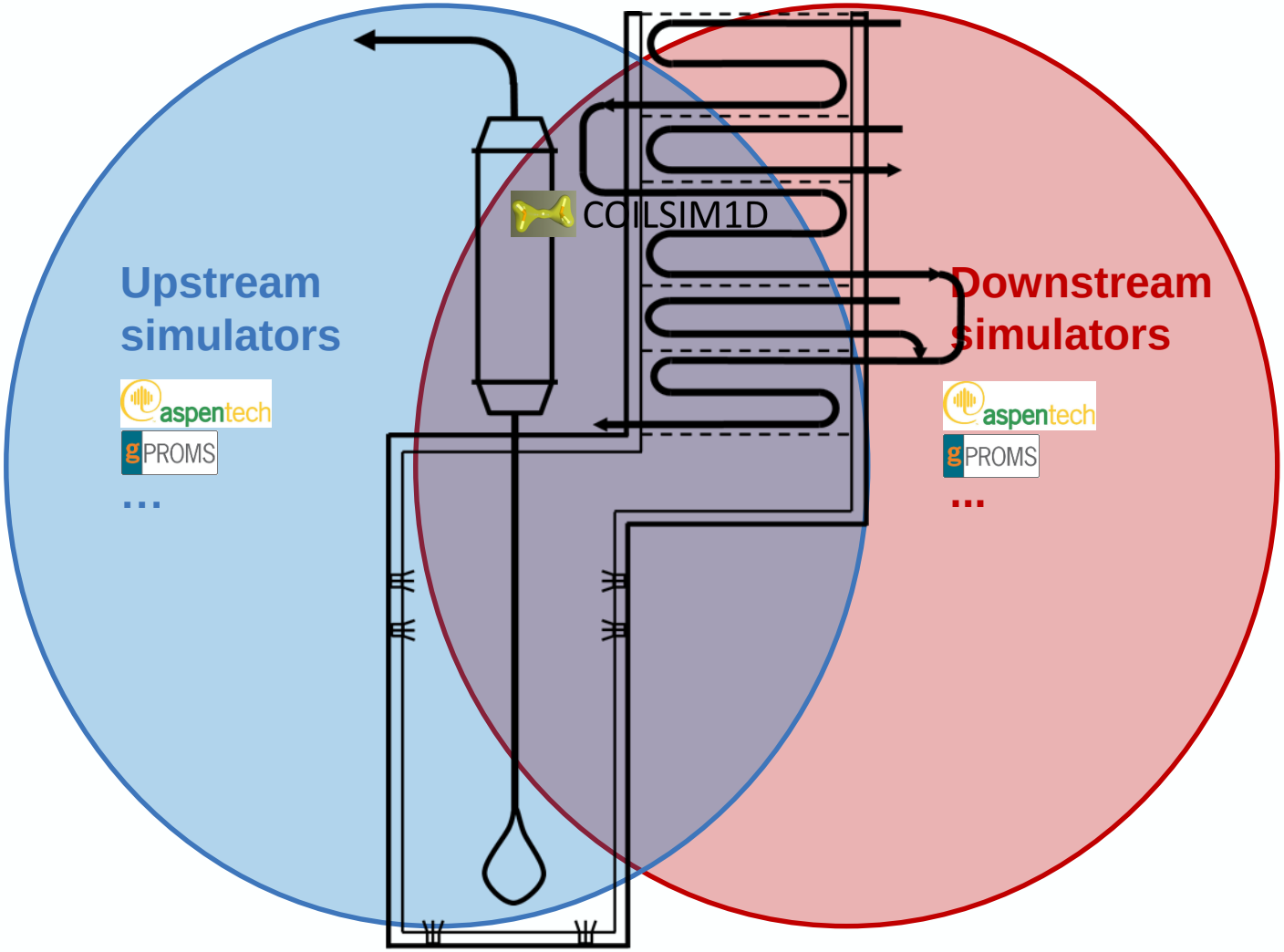
First there was a coil…



COILSIM1D



… and now the entire plant



Outline

- Introduction
- COILSIM1D: The Simulation Package
- New Features of COILSIM1D
- I/O files and Interfacing
- Conclusions

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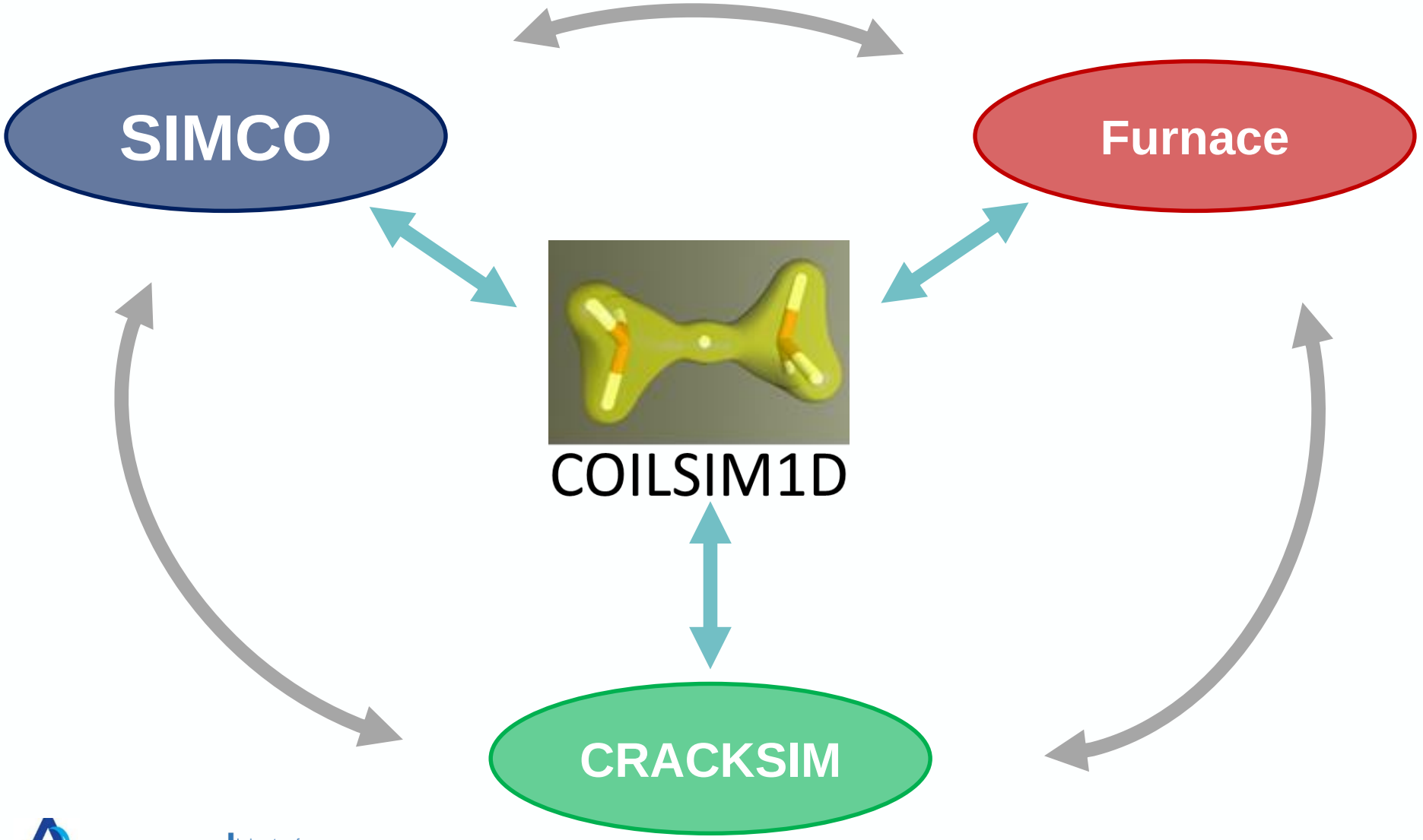
Key elements of COILSIM

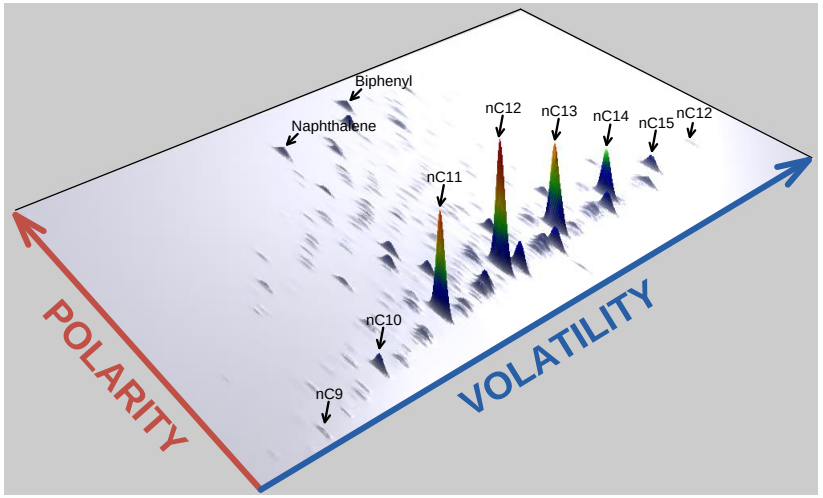


SIMCO: Feedstock Reconstruction

- A detailed model requires a detailed molecular composition

Bulk properties / Commercial indices

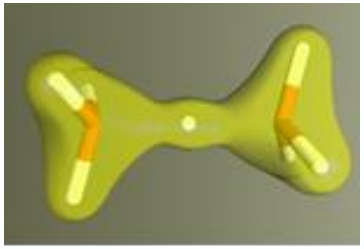
- Gaseous feeds
- Naphthas
- Gas condensates
- Kerosene
- HVGO
- VGO
- …



Validation by means of GCxGC

SIMCO

Molecular feed composition



COILSIM1D

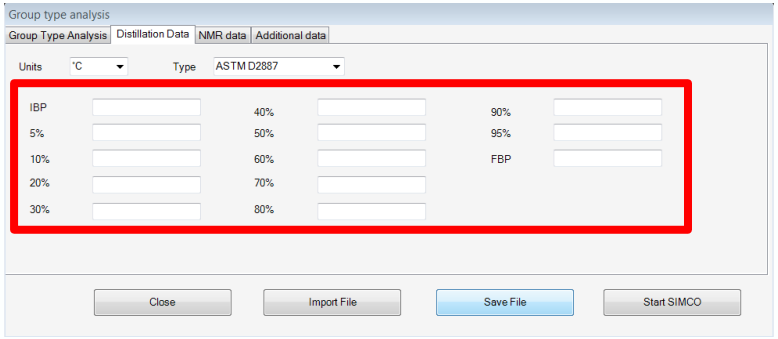
Detailed product distribution

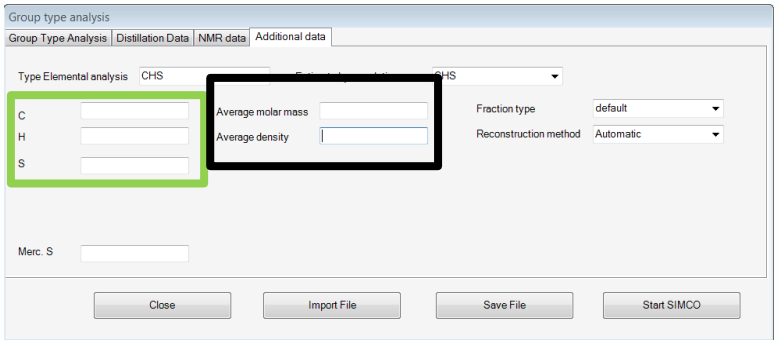
SIMCO: Feedstock Reconstruction

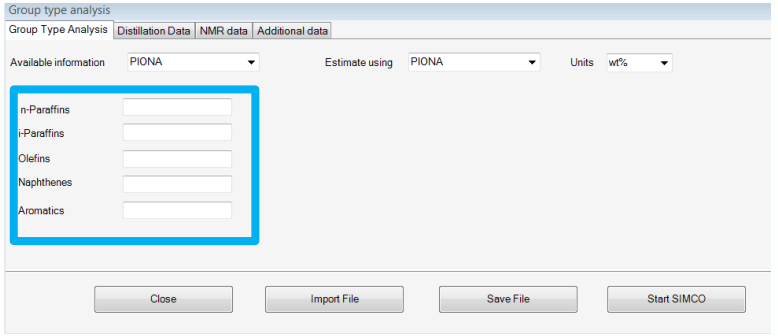
Input given via the GUI

Bulk properties :

- Average Molecular Weight
- Specific Density
- Elemental analysis
- PIONA
- Distillation data
  - TBP
  - ASTM D86
  - ASTM D2887







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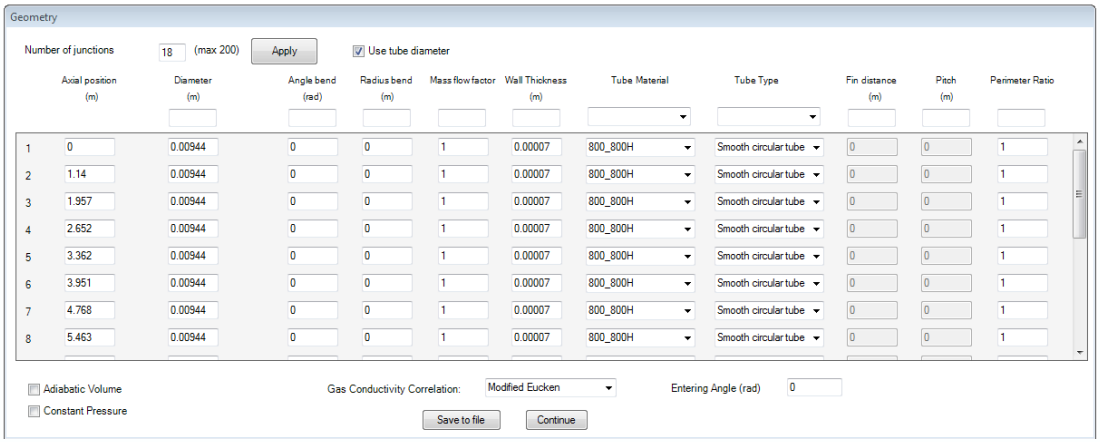
Reactor definition

- Built-in library of commercial coil geometries
- 'New coil Geometry' tool:



- Dedicated correlations for enhanced heat transfer of 3D geometries:

$$\boldsymbol{Nu_D} = 0.242\ Re_D^{0.645}\ Pr^{0.4} \left(\frac{P}{D_e}\right)^{-2.95\ Re_D^{-0.23}} \left(\frac{B}{D_e}\right)^{0.0045\ Re_D^{0.31}} \left(\frac{T}{T_w}\right)^{0.5}$$

$$\boldsymbol{Nu_D} = 4.11\ Re_D^{0.326}\ Pr^{0.4} \left(\frac{P}{D_e}\right)^{-1.4\ 10^{-6}\ Re_D^{1.07}} \left(\frac{D_i}{D_e}\right)$$

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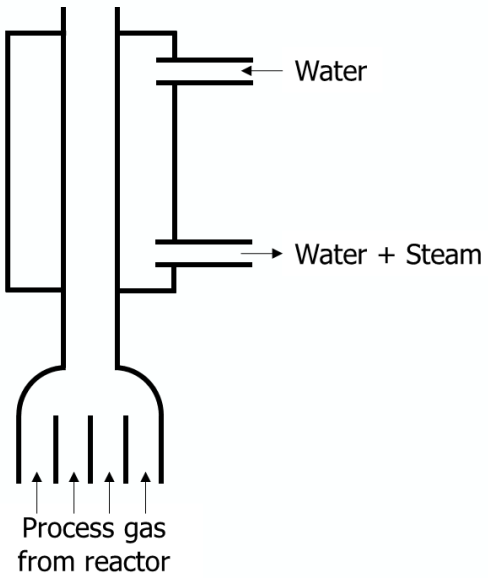
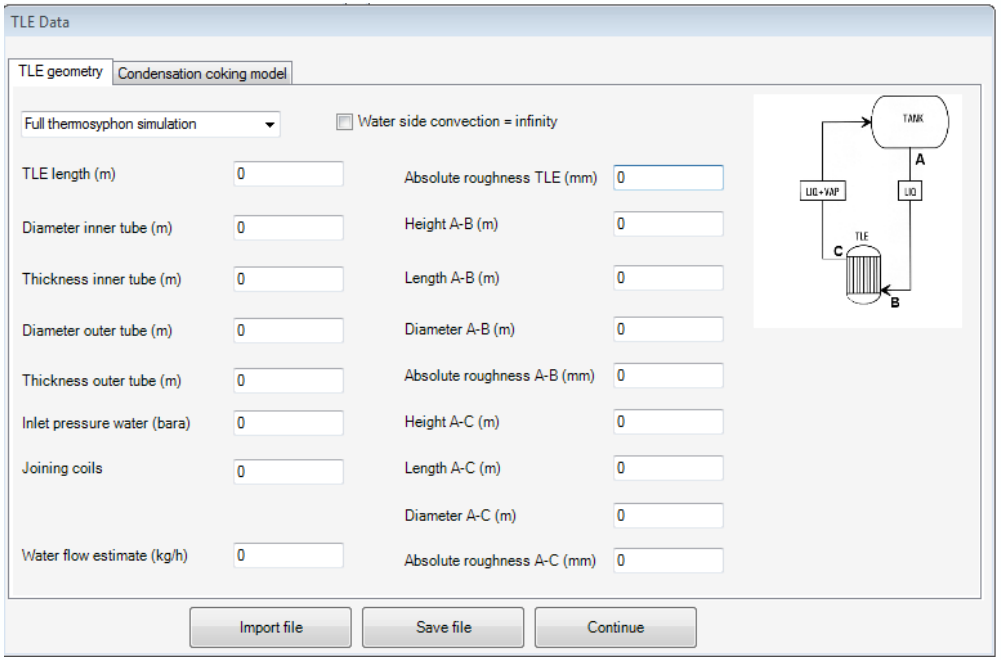
Transfer Line Exchanger

- Various boundary conditions
- Dedicated condensation coke model

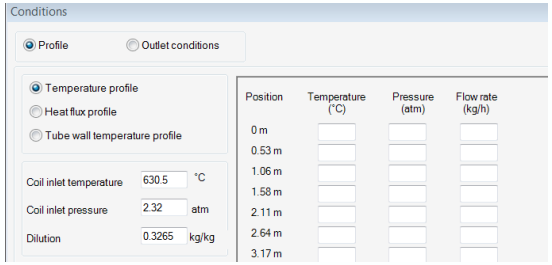




Simulation Strategies

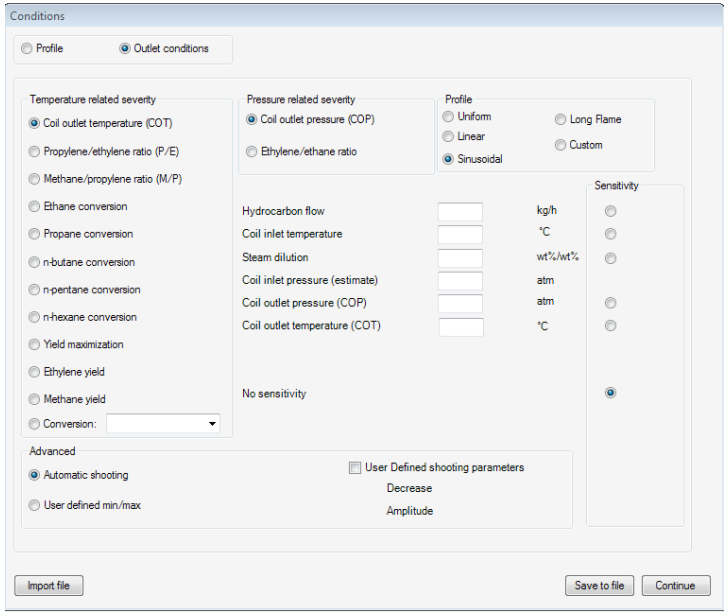
Profiles:

- Process gas temperature
- Tube wall temperature
- Heat flux to coil



Outlet conditions:

- Common severity indices
- Yield maximization
- Sensitivity analyses



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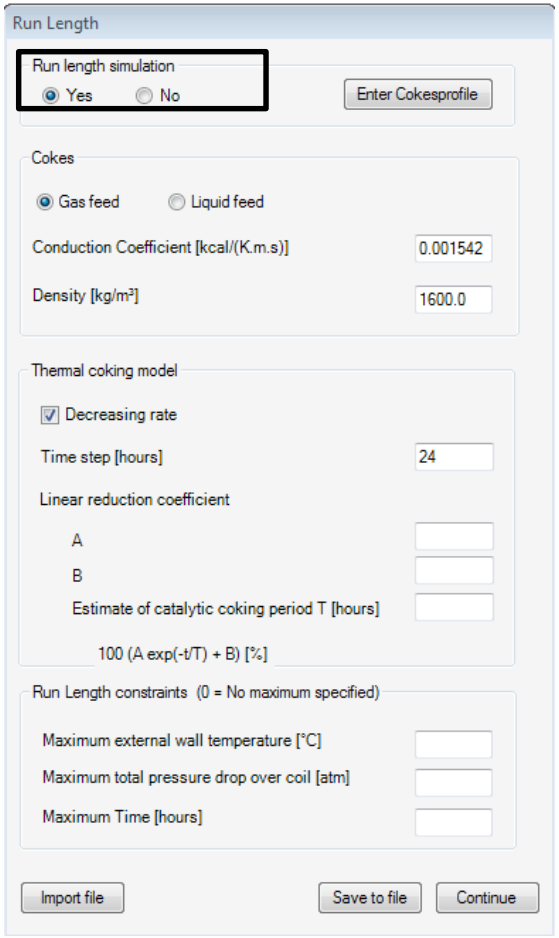
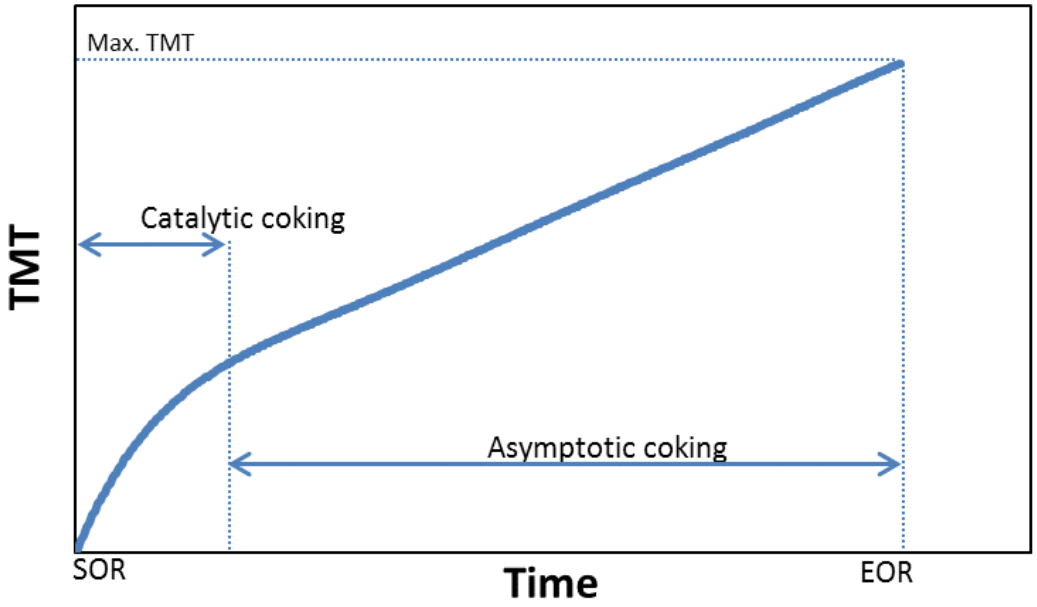
Simulation Strategies: Run length



Run length simulation:

- Dedicated radical coking models
  - Catalytic regime can be included
- User-defined max TMT and/or max ΔP



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- New Features of COILSIM1D
- I/O files and Interfacing
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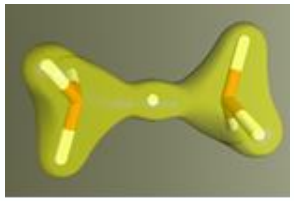
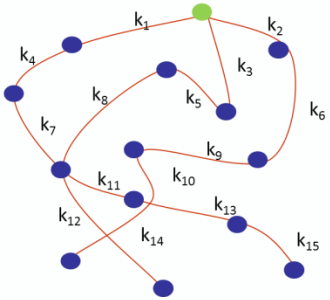
Kinetic Model for Steam Cracking



COILSIM1D

Kinetic model



1D reactor model

- Broadest kinetic model for steam cracking
  - 720+ molecules
  - 43 radicals
  - 300,000+ reactions
- Based on high level Ab initio data, and kinetics re-fitted with experimental data (pilot and industrial)

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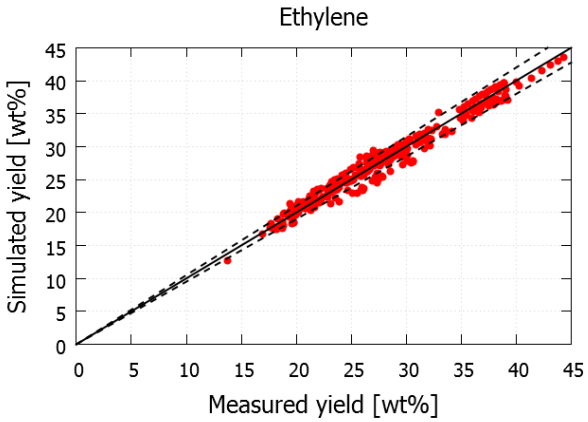
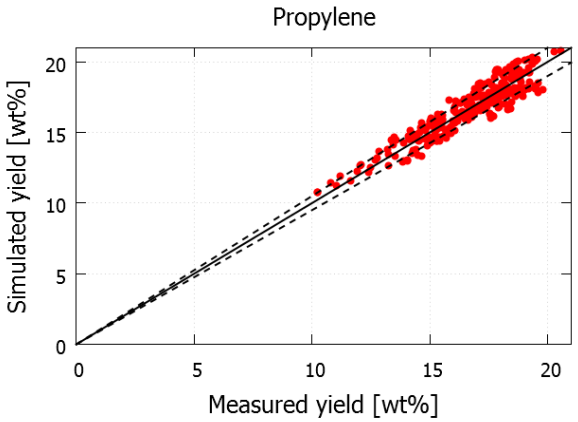
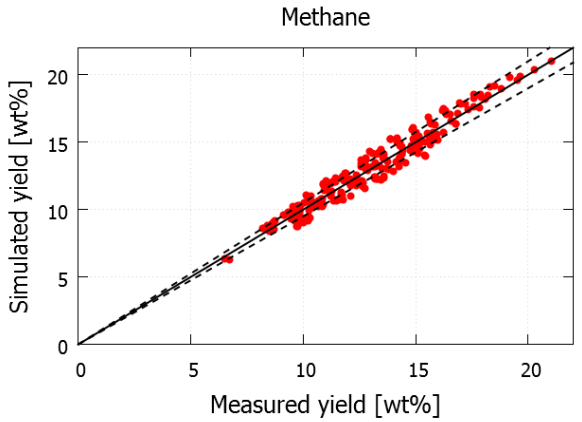
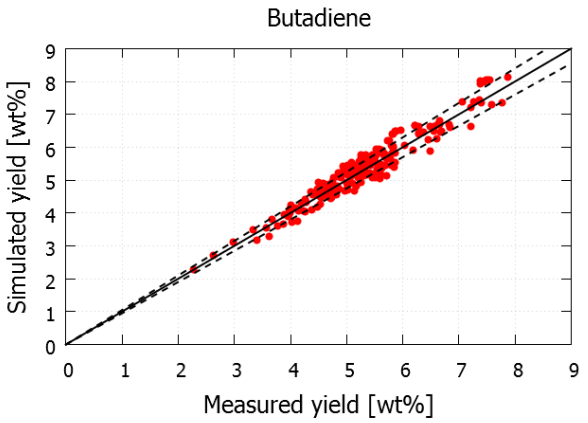
Kinetic Model for Steam Cracking

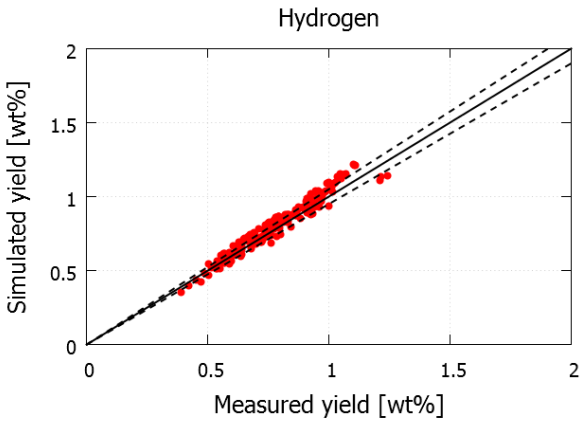
- Extended to include oxygenates
- Validated with an extensive data set

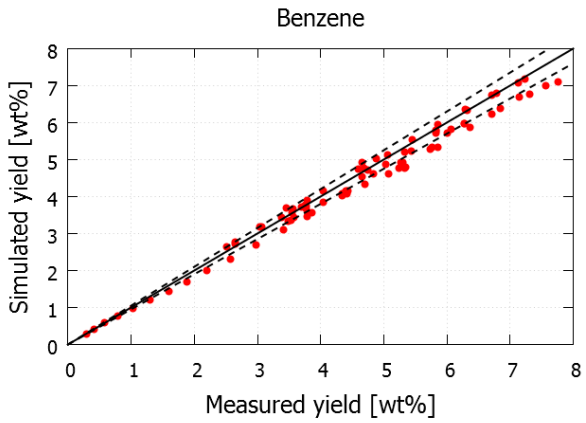












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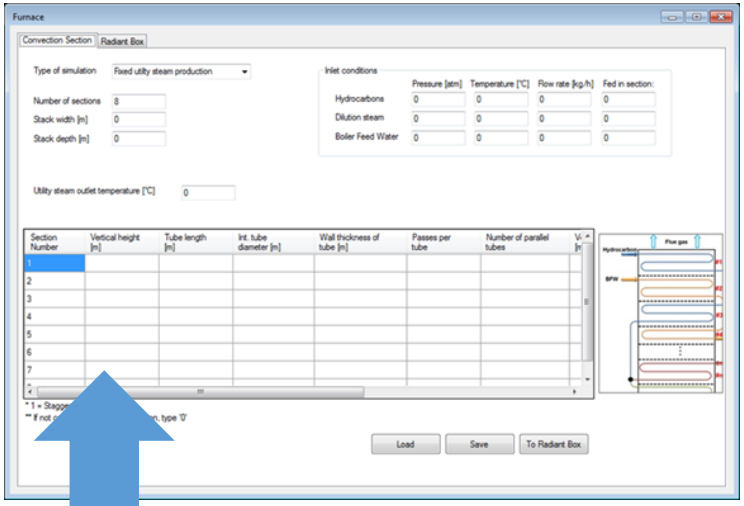
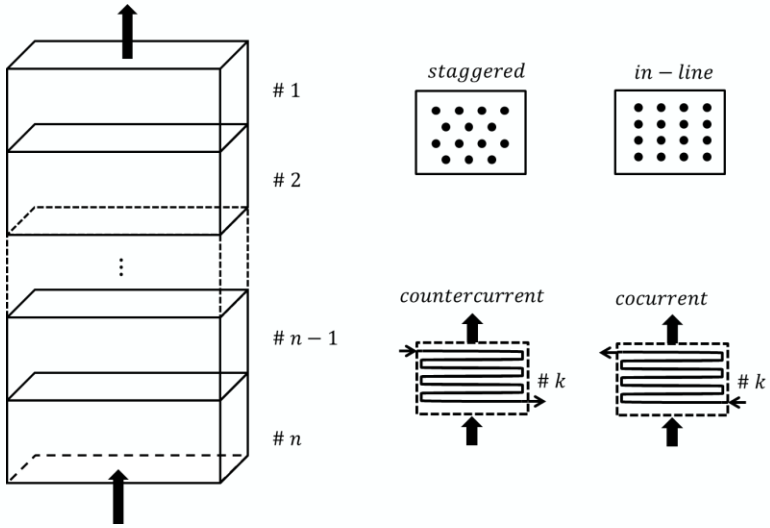
Convection Section Model

- Dedicated evaporation model
- Various configurations and tube materials supported



Geometry
Process streams
Flue gas side
Feed composition



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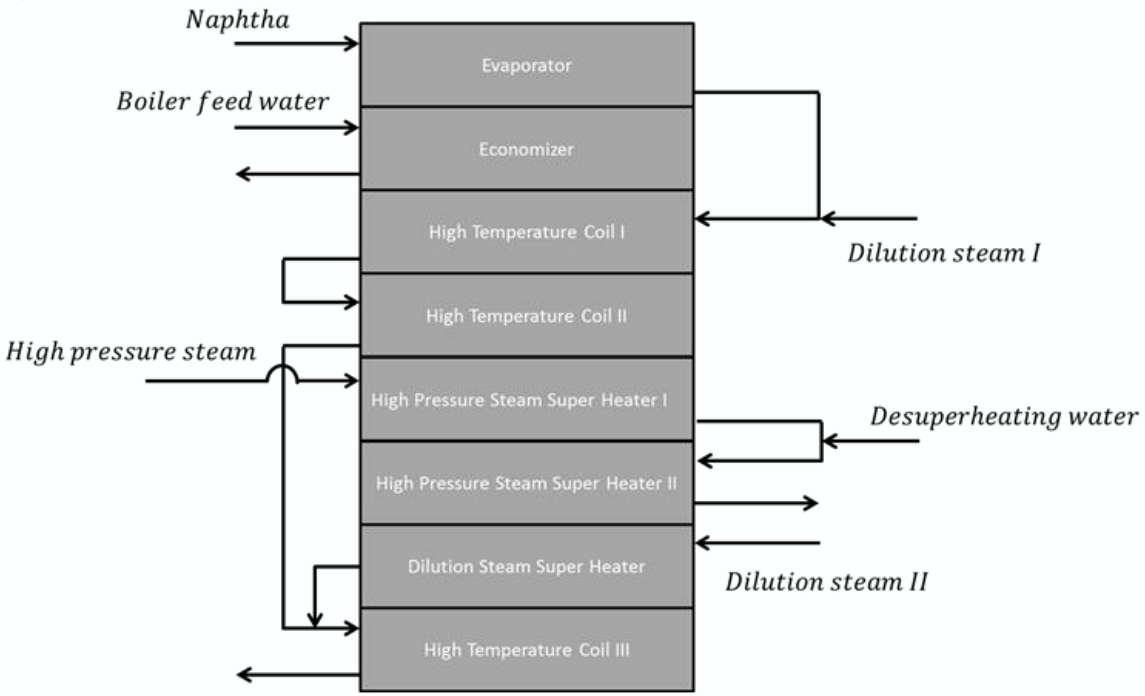
Convection Section Model

Illustrative case

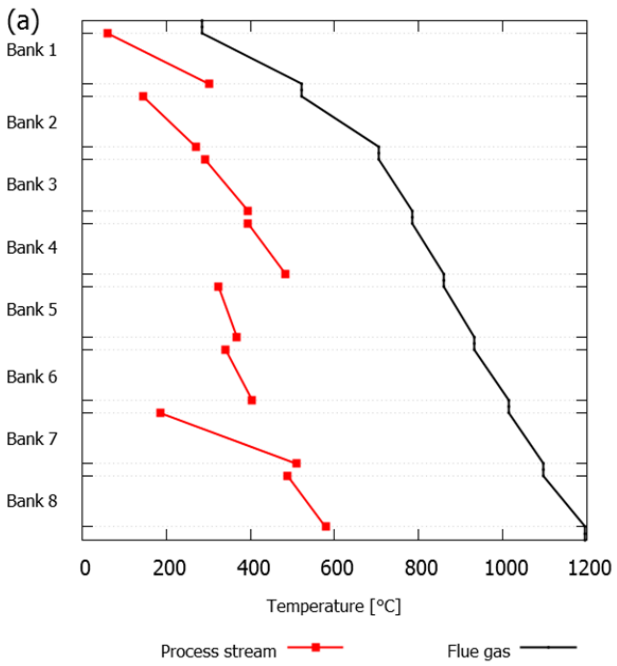
- Liquid feed, SIMCO reconstructed
- 72 different components
- Different mixing points

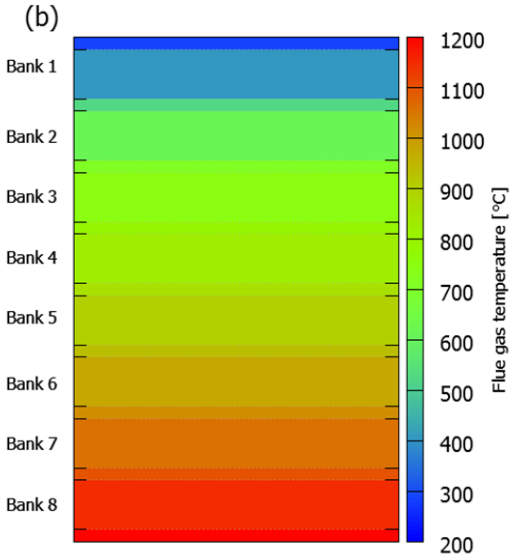
Commercial indices of the naphtha feed	
density [kg/m³]	708.8
ASTM D86 [°C]	
IBP	39
50%	99
FBP	165
PIONA [wt%]	
Paraffin's	36.5
Iso-paraffin's	32.8
Olefins	0.0
Naphtenes	21.4
Aromatics	9.20



Convection Section Model

Demonstration case : Results





Bank name	Duty pick up [MW]
Evaporator	7.28
Economizer	5.95
HTC 1	2.65
HTC 2	2.53
HPSS 1	2.48
HPSS 2	2.78
DSSH	2.89
HTC3	3.53

CIT : 580 °C

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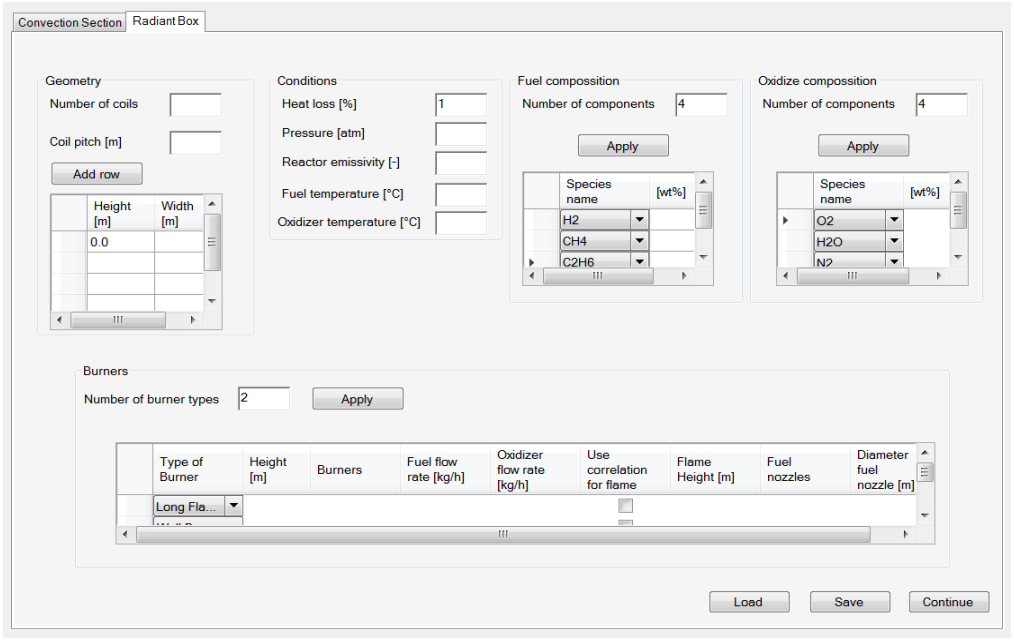
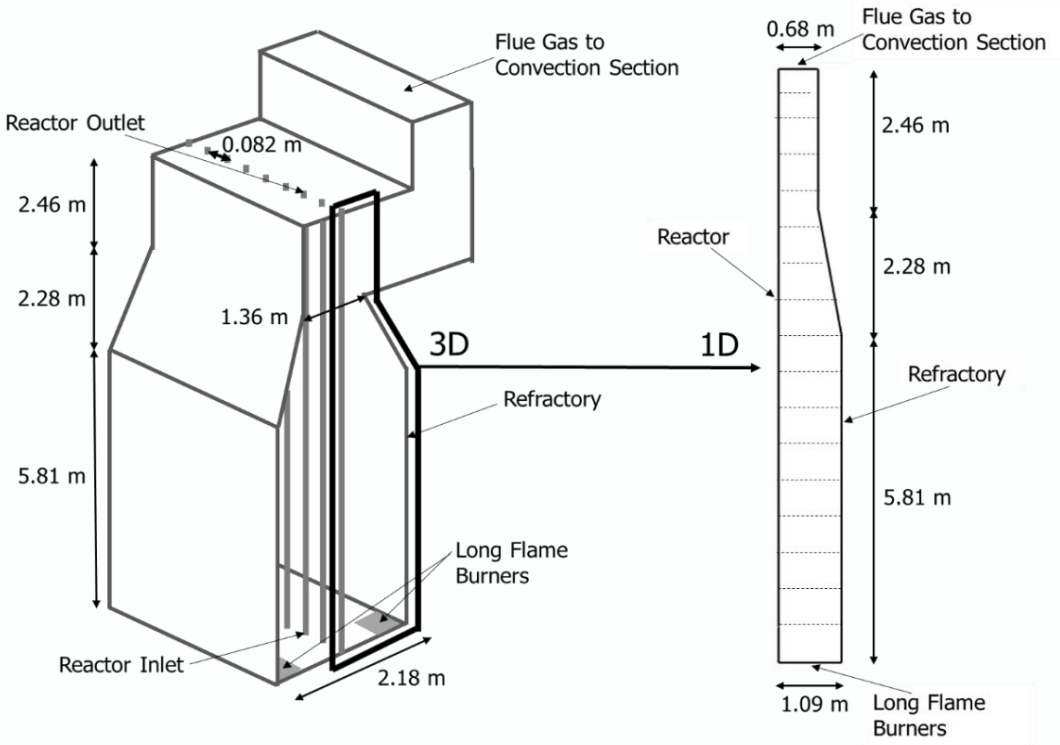
Firebox Simulation Model

- Flexible model:
  - Geometry
  - Fuel composition
  - Various input conditions
  - Burner arrangements



Firebox, Reactor and TLE Simulation

- **Illustrative Millisecond case:**



Feed: 118.5 kg C_3H_8 / h

Dilution: 0.33 kg / kg

CIT: 630.5 °C

CIP: 2.35 bara

Fuel: 53.9 kg CH_4 / h

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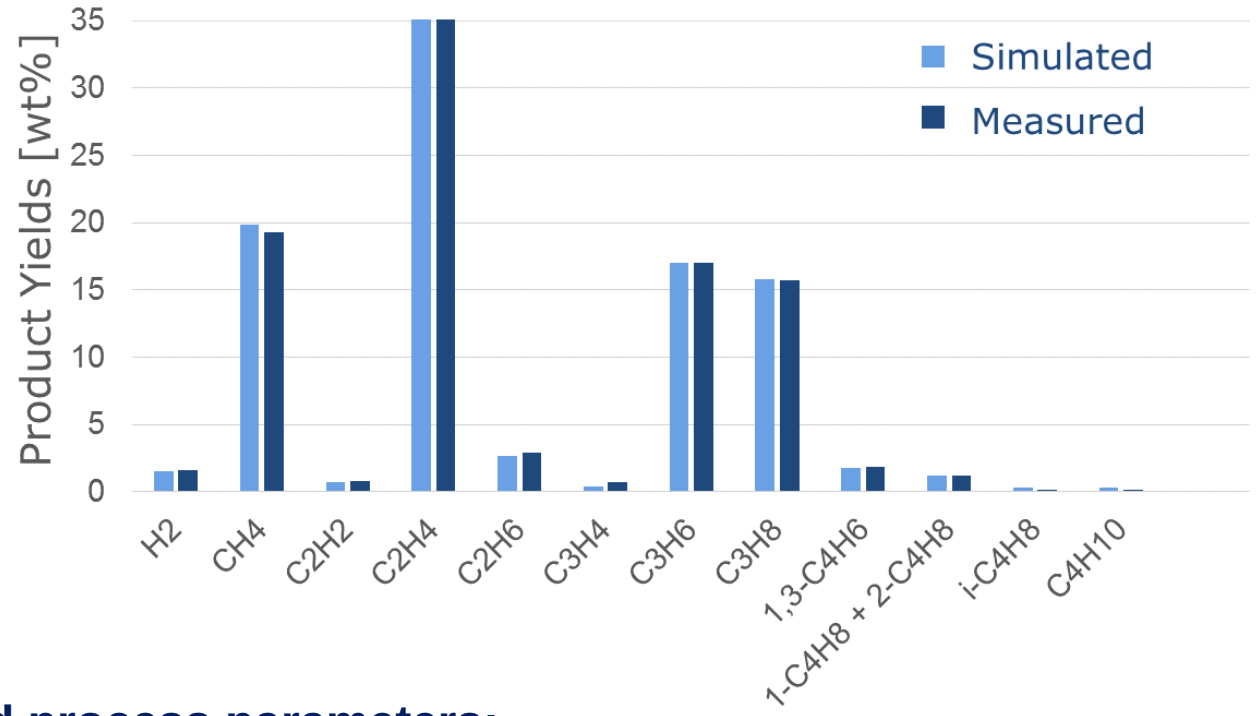
Firebox, Reactor and TLE Simulation



Simulated process parameters:

COT: 879 °C
TLE outlet T: 446 °C
Furnace efficiency: 43.2 %
Bridge-wall temperature: 1138 °C

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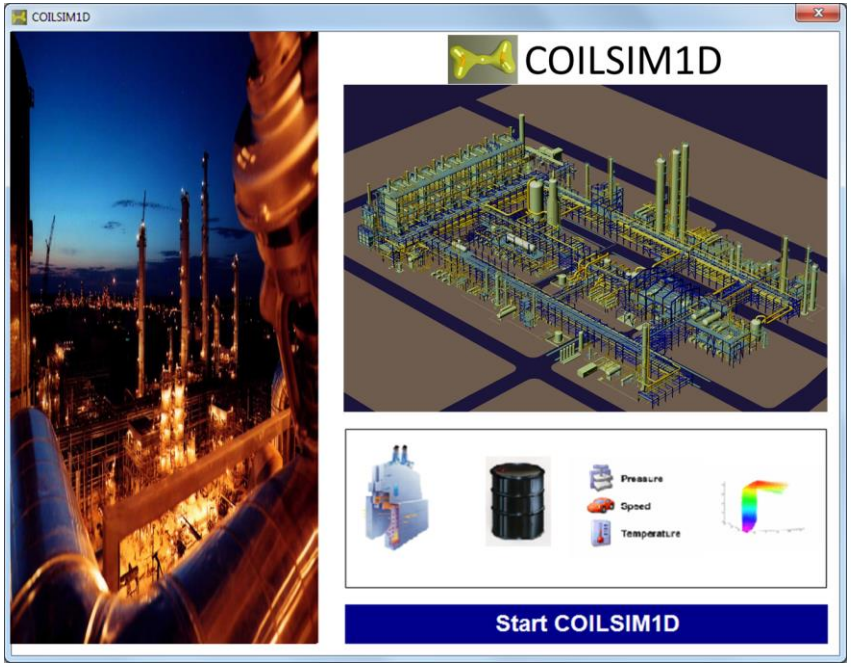
I/O files and interfacing

- Easy interaction with other software
- Human/machine readable I/O files:
  -Scripts for creation and result retrieval of simulations.



nafta.i - SciTE

File Edit Search View Tools Options Language Buffers Help

1 nafta.i

```
 72
0.01997 015 1 !n-C4H10
0.05148 028 0 !iso_C5
0.09647 029 1 !n_C5
0.00655 040 0 !cyC5
0.01810 043 0 !mcyC5
0.02038 046 0 !cyC6
0.03870 049 0 !mcyC6
0.03124 052 0 !t1.3dmcyC6
0.00347 055 0 !etcyC6
0.00988 060 0 !benzene
0.01726 061 0 !toluene
0.02474 062 0 !xylene
0.00452 063 0 !etBenzene
0.01606 065 0 !iP-C9aro
0.04443 074 0 !C6_2mip
0.08069 243 1 !C6_npar
0.06355 244 1 !C7_npar
0.05286 245 1 !C8_npar
0.03813 246 1 !C9_npar
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0.02222 275 0 !C6_3mip
0.01611 276 0 !C7_3mip
0.01338 277 0 !C8_3mip
0.01254 278 0 !C9_3mip
0.00795 279 0 !C10_3mip
```

li=1 co=1 INS (CR+LF)

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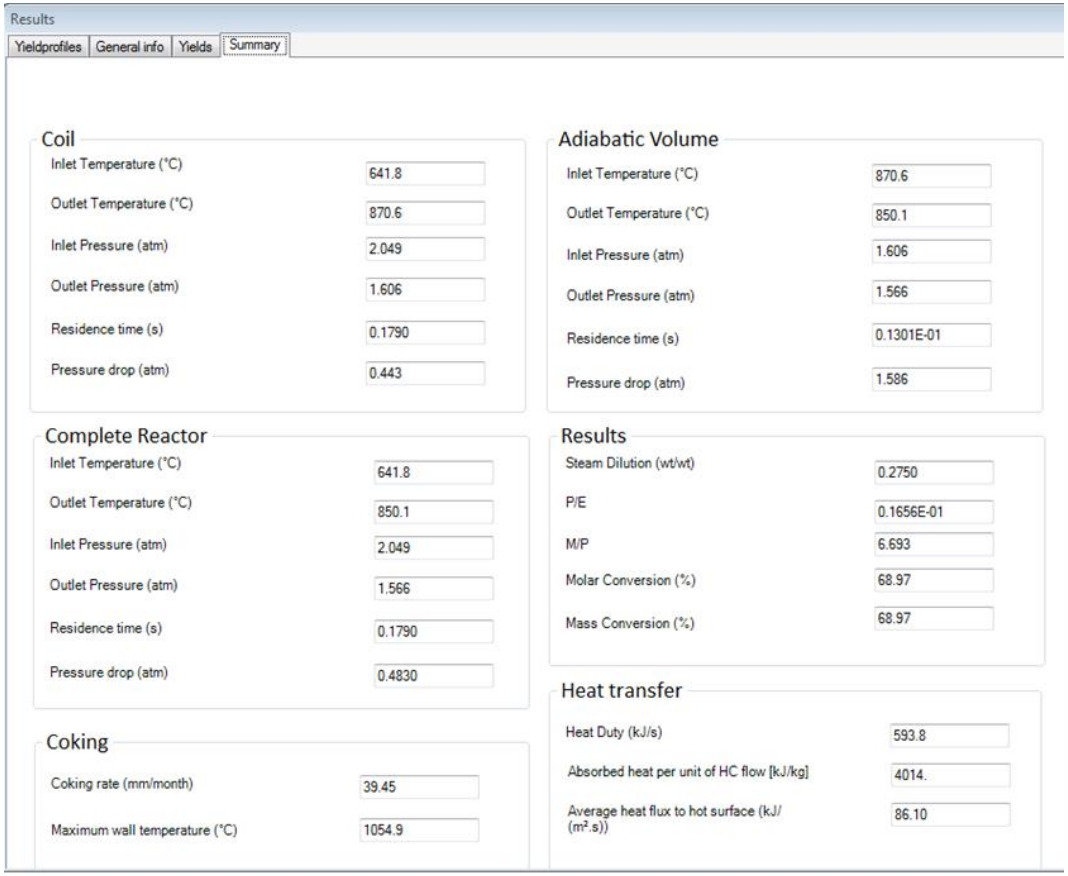
I/O files and interfacing

Summary of main results displayed in GUI:



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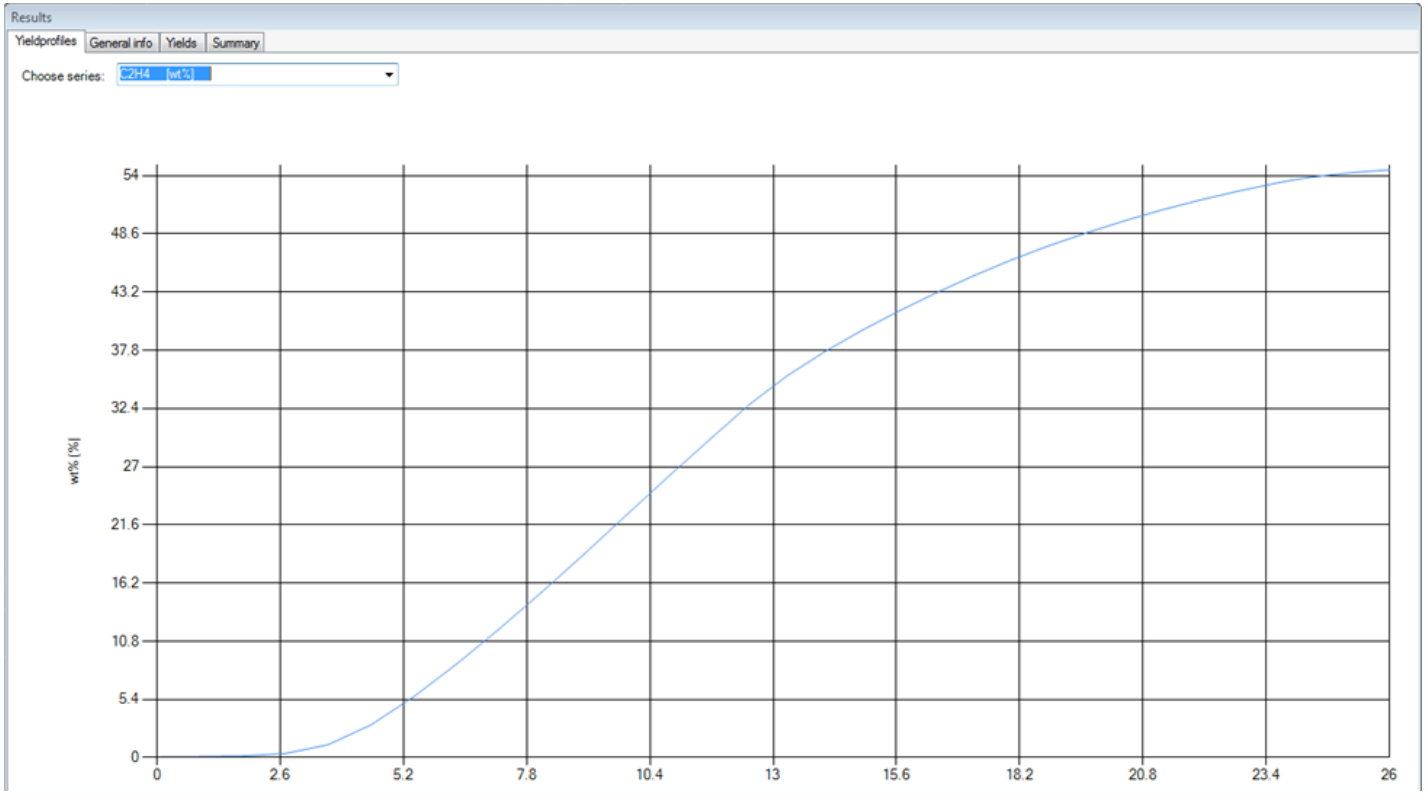
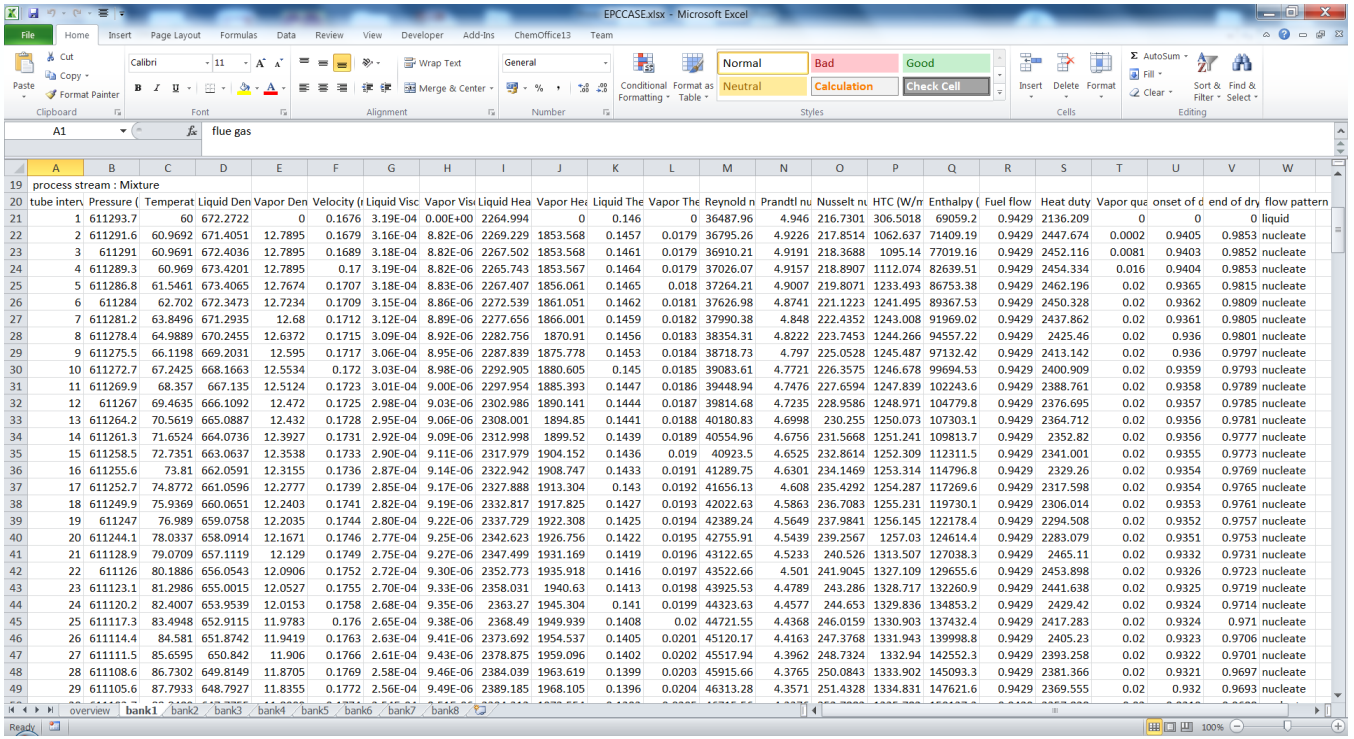
I/O files and interfacing

Plots for rapid result evaluation in GUI:



I/O files and interfacing

- Detailed result (output) files
- Easy to import in spread sheets



	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	T	U	V	W
19	process stream : Mixture																						
20	tube interv	Pressure (	Temperat	Liquid Den	Vapor Den	Velocity (r	Liquid Visc	Vapor Visc	Liquid Hea	Vapor Hea	Liquid The	Vapor The	Reynold n	Prandtl nu	Nusselt nu	HTC (W/m	Enthalpy (	Fuel flow	Heat duty	Vapor que	onset of d	end of dry	flow pattern
21	1	611293.7	60	672.2722	0	0.1676	3.19E-04	0.00E+00	2264.994	0	0.146	0	36487.96	4.946	216.7301	306.5018	69059.2	0.9429	2136.209	0	0	0	liquid
22	2	611291.6	60.9692	671.4051	12.7895	0.1679	3.16E-04	8.82E-06	2269.229	1853.568	0.1457	0.0179	36795.26	4.9226	217.8514	1062.637	71409.19	0.9429	2447.674	0.0002	0.9405	0.9853	nucleate
23	3	611291	60.9691	672.4036	12.7895	0.1689	3.18E-04	8.82E-06	2267.502	1853.568	0.1461	0.0179	36910.21	4.9191	218.3688	1095.14	77019.16	0.9429	2452.116	0.0081	0.9403	0.9852	nucleate
24	4	611289.3	60.969	673.4201	12.7895	0.17	3.19E-04	8.82E-06	2265.743	1853.567	0.1464	0.0179	37026.07	4.9157	218.8907	1112.074	82639.51	0.9429	2454.334	0.016	0.9404	0.9853	nucleate
25	5	611286.8	61.5461	673.4065	12.7674	0.1707	3.18E-04	8.83E-06	2267.407	1856.061	0.1465	0.018	37264.21	4.9007	219.8071	1233.493	86753.38	0.9429	2462.196	0.02	0.9365	0.9815	nucleate
26	6	611284	62.702	672.3473	12.7234	0.1709	3.15E-04	8.86E-06	2272.539	1861.051	0.1462	0.0181	37626.98	4.8741	221.1223	1241.495	89367.53	0.9429	2450.328	0.02	0.9362	0.9809	nucleate
27	7	611281.2	63.8496	671.2935	12.68	0.1712	3.12E-04	8.89E-06	2277.656	1866.001	0.1459	0.0182	37990.38	4.848	222.4352	1243.008	91969.02	0.9429	2437.862	0.02	0.9361	0.9805	nucleate
28	8	611278.4	64.9889	670.2455	12.6372	0.1715	3.09E-04	8.92E-06	2282.756	1870.91	0.1456	0.0183	38354.31	4.8222	223.7453	1244.266	94557.22	0.9429	2425.46	0.02	0.936	0.9801	nucleate
29	9	611275.5	66.1198	669.2031	12.595	0.1717	3.06E-04	8.95E-06	2287.839	1875.778	0.1453	0.0184	38718.73	4.797	225.0528	1245.487	97132.42	0.9429	2413.142	0.02	0.936	0.9797	nucleate
30	10	611272.7	67.2425	668.1663	12.5534	0.172	3.03E-04	8.98E-06	2292.905	1880.605	0.145	0.0185	39083.61	4.7721	226.3575	1246.678	99694.53	0.9429	2400.909	0.02	0.9359	0.9793	nucleate
31	11	611269.9	68.357	667.135	12.5124	0.1723	3.01E-04	9.00E-06	2297.954	1885.393	0.1447	0.0186	39448.94	4.7476	227.6594	1247.839	102243.6	0.9429	2388.761	0.02	0.9358	0.9789	nucleate
32	12	611267	69.4635	666.1092	12.472	0.1725	2.98E-04	9.03E-06	2302.986	1890.141	0.1444	0.0187	39814.68	4.7235	228.9586	1248.971	104779.8	0.9429	2376.695	0.02	0.9357	0.9785	nucleate
33	13	611264.2	70.5619	665.0887	12.432	0.1728	2.95E-04	9.06E-06	2308.001	1894.85	0.1441	0.0188	40180.83	4.6998	230.255	1250.073	107303.1	0.9429	2364.712	0.02	0.9356	0.9781	nucleate
34	14	611261.3	71.6524	664.0736	12.3927	0.1731	2.92E-04	9.09E-06	2312.998	1899.52	0.1439	0.0189	40554.96	4.6756	231.5668	1251.241	109813.7	0.9429	2352.82	0.02	0.9356	0.9777	nucleate
35	15	611258.5	72.7351	663.0637	12.3538	0.1733	2.90E-04	9.11E-06	2317.979	1904.152	0.1436	0.019	40923.5	4.6525	232.8614	1252.309	112311.5	0.9429	2341.001	0.02	0.9355	0.9773	nucleate
36	16	611255.6	73.81	662.0591	12.3155	0.1736	2.87E-04	9.14E-06	2322.942	1908.747	0.1433	0.0191	41289.75	4.6301	234.1469	1253.314	114796.8	0.9429	2329.26	0.02	0.9354	0.9769	nucleate
37	17	611252.7	74.8772	661.0596	12.2777	0.1739	2.85E-04	9.17E-06	2327.888	1913.304	0.143	0.0192	41656.13	4.608	235.4292	1254.287	117269.6	0.9429	2317.598	0.02	0.9354	0.9765	nucleate
38	18	611249.9	75.9369	660.0651	12.2403	0.1741	2.82E-04	9.19E-06	2332.817	1917.825	0.1427	0.0193	42022.63	4.5863	236.7083	1255.231	119730.1	0.9429	2306.014	0.02	0.9353	0.9761	nucleate
39	19	611247	76.989	659.0758	12.2035	0.1744	2.80E-04	9.22E-06	2337.729	1922.308	0.1425	0.0194	42389.24	4.5649	237.9841	1256.145	122178.4	0.9429	2294.508	0.02	0.9352	0.9757	nucleate
40	20	611244.1	78.0337	658.0914	12.1671	0.1746	2.77E-04	9.25E-06	2342.623	1926.756	0.1422	0.0195	42755.91	4.5439	239.2567	1257.03	124614.4	0.9429	2283.079	0.02	0.9351	0.9753	nucleate
41	21	611128.9	79.0709	657.1119	12.129	0.1749	2.75E-04	9.27E-06	2347.499	1931.169	0.1419	0.0196	43122.65	4.5233	240.526	1313.507	127038.3	0.9429	2465.11	0.02	0.9332	0.9731	nucleate
42	22	611126	80.1886	656.0543	12.0906	0.1752	2.72E-04	9.30E-06	2352.773	1935.918	0.1416	0.0197	43522.66	4.501	241.9045	1327.109	129655.6	0.9429	2453.898	0.02	0.9326	0.9723	nucleate
43	23	611123.1	81.2986	655.0015	12.0527	0.1755	2.70E-04	9.33E-06	2358.031	1940.63	0.1413	0.0198	43925.53	4.4789	243.286	1328.717	132260.9	0.9429	2441.638	0.02	0.9325	0.9719	nucleate
44	24	611120.2	82.4007	653.9539	12.0153	0.1758	2.68E-04	9.35E-06	2363.27	1945.304	0.141	0.0199	44323.63	4.4577	244.653	1329.836	134853.2	0.9429	2429.42	0.02	0.9324	0.9714	nucleate
45	25	611117.3	83.4948	652.9115	11.9783	0.176	2.65E-04	9.38E-06	2368.49	1949.939	0.1408	0.02	44721.55	4.4368	246.0159	1330.903	137432.4	0.9429	2417.283	0.02	0.9324	0.971	nucleate
46	26	611114.4	84.581	651.8742	11.9419	0.1763	2.63E-04	9.41E-06	2373.692	1954.537	0.1405	0.0201	45120.17	4.4163	247.3768	1331.943	139998.8	0.9429	2405.23	0.02	0.9323	0.9706	nucleate
47	27	611111.5	85.6595	650.842	11.906	0.1766	2.61E-04	9.43E-06	2378.875	1959.096	0.1402	0.0202	45517.94	4.3962	248.7324	1332.94	142552.3	0.9429	2393.258	0.02	0.9322	0.9701	nucleate
48	28	611108.6	86.7302	649.8149	11.8705	0.1769	2.58E-04	9.46E-06	2384.039	1963.619	0.1399	0.0203	45915.66	4.3765	250.0843	1333.902	145093.3	0.9429	2381.366	0.02	0.9321	0.9697	nucleate
49	29	611105.6	87.7933	648.7927	11.8355	0.1772	2.56E-04	9.49E-06	2389.185	1968.105	0.1396	0.0204	46313.28	4.3571	251.4328	1334.831	147621.6	0.9429	2369.555	0.02	0.932	0.9693	nucleate

AVGI

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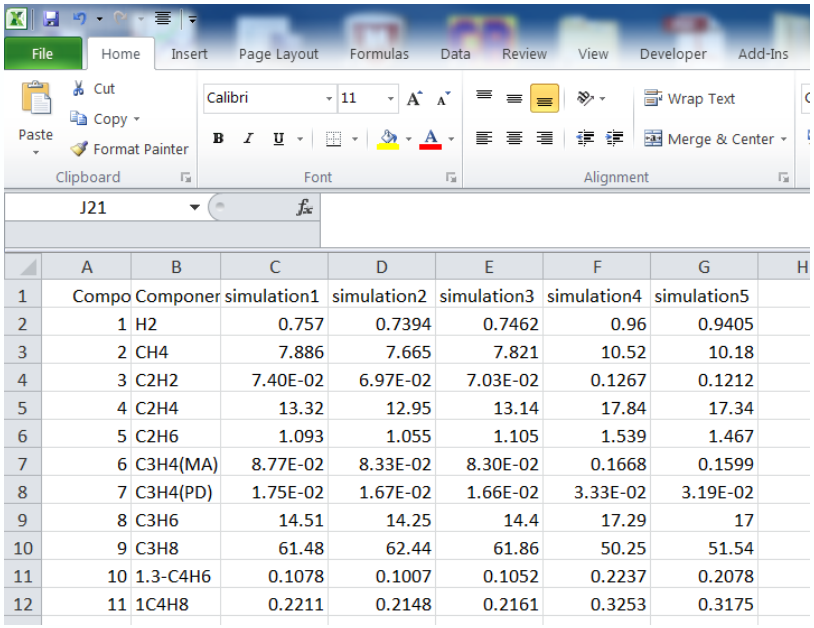
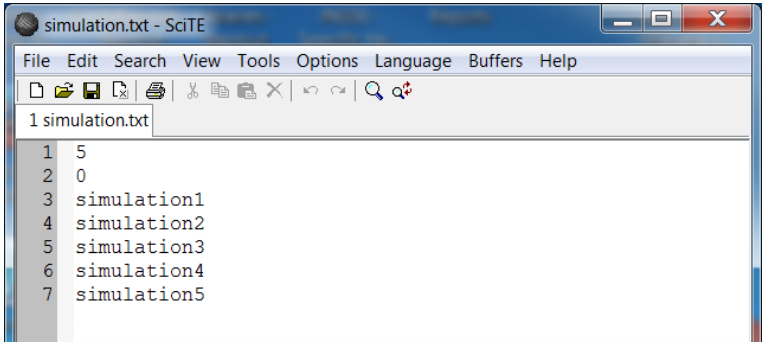
I/O files and interfacing

Batch simulations:

- Manual (via GUI)
- Automated (via code scripts)



	A	B	C	D	E	F	G
1	Compo	Componer	simulation1	simulation2	simulation3	simulation4	simulation5
2	1	H2	0.757	0.7394	0.7462	0.96	0.9405
3	2	CH4	7.886	7.665	7.821	10.52	10.18
4	3	C2H2	7.40E-02	6.97E-02	7.03E-02	0.1267	0.1212
5	4	C2H4	13.32	12.95	13.14	17.84	17.34
6	5	C2H6	1.093	1.055	1.105	1.539	1.467
7	6	C3H4(MA)	8.77E-02	8.33E-02	8.30E-02	0.1668	0.1599
8	7	C3H4(PD)	1.75E-02	1.67E-02	1.66E-02	3.33E-02	3.19E-02
9	8	C3H6	14.51	14.25	14.4	17.29	17
10	9	C3H8	61.48	62.44	61.86	50.25	51.54
11	10	1.3-C4H6	0.1078	0.1007	0.1052	0.2237	0.2078
12	11	1C4H8	0.2211	0.2148	0.2161	0.3253	0.3175



Clear overview of performed simulations

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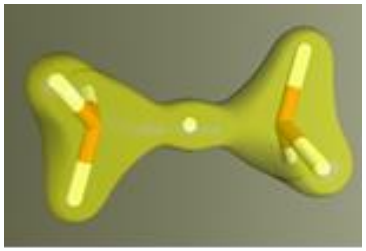
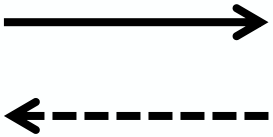
I/O files and interfacing

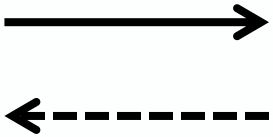
Global plant optimization



COILSIM1D



Interface



aspentech

gPROMS

Interface:

- Translation of molecule names
- Extraction of process conditions
- Coordination of the interaction

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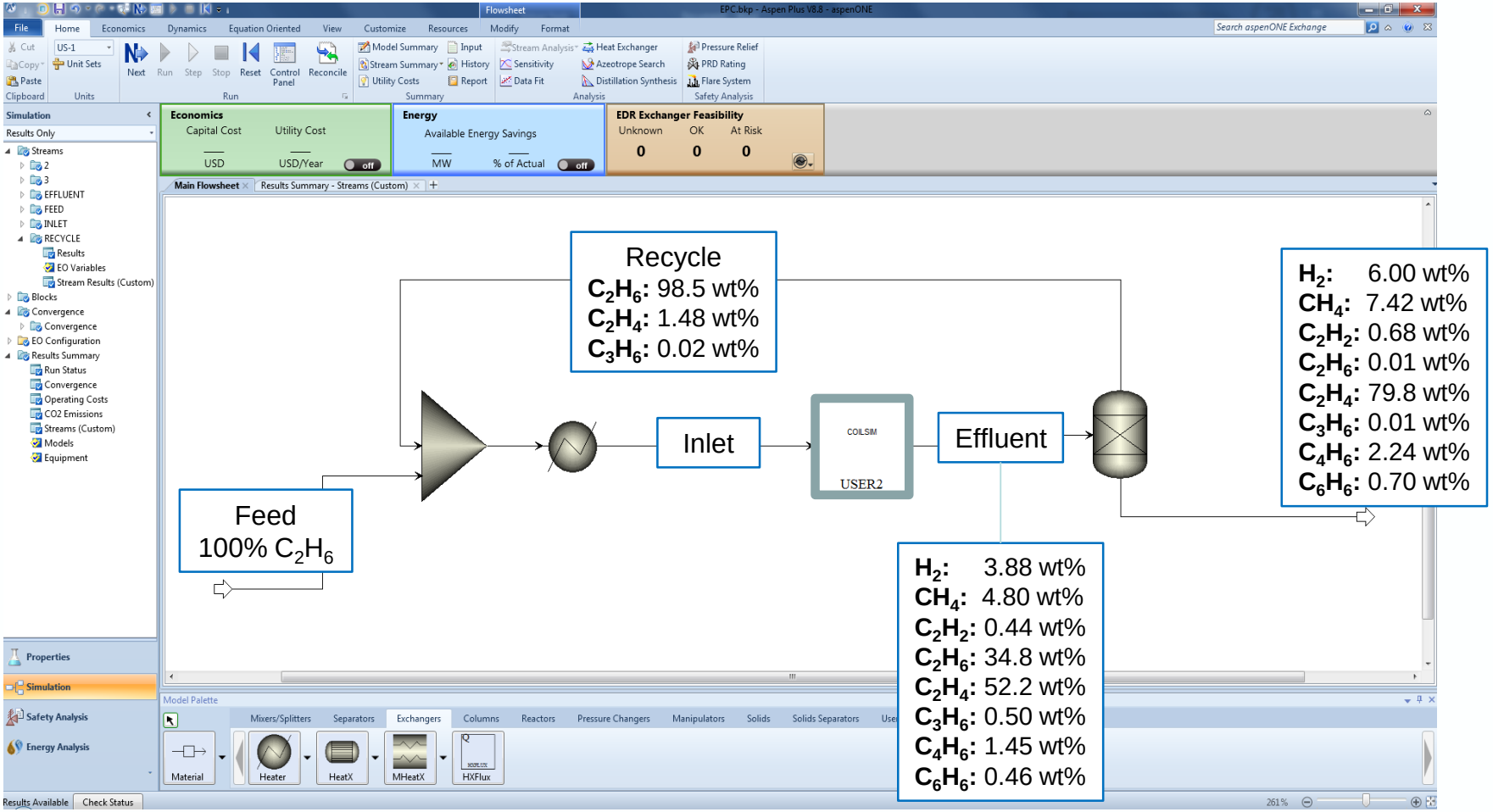
I/O files and interfacing

Example: C_2H_6 cracker case (incl. recycle) with Aspen Plus®

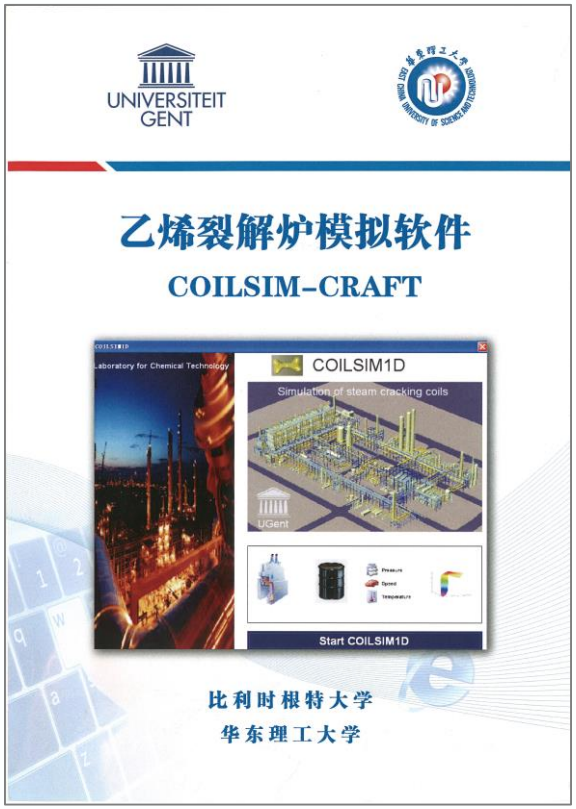


I/O files and interfacing

RTO

- Demonstration case carried out at demonstration unit in China

- Integration in an external package for control of the unit



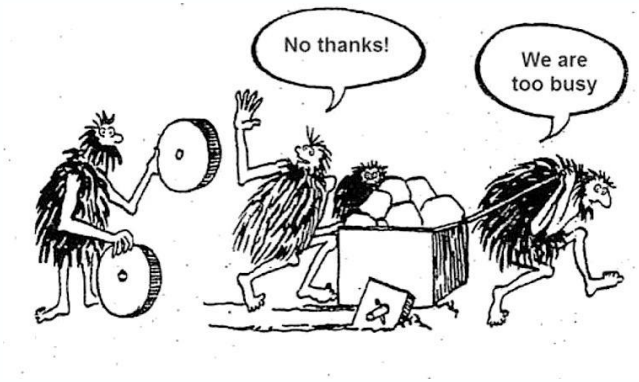
Outline

- Introduction
- COILSIM1D: The Simulation Package
- New Features of COILSIM1D
- I/O files and Interfacing
- Conclusions

Wrapping up

- COILSIM1D can now simulate entire furnaces, all in one package, with one click
- Flexible, user-friendly and accurate simulations
- Easy interaction with third-party software

Questions?


No thanks!
We are too busy


WHAT DO YOU MEAN WE HAVE TO CHANGE???
WE'VE ALWAYS DONE IT THIS WAY
memegenerator.net


We do it this way because we've always done it this way, son!