

192F

FULL FURNACE SIMULATIONS AND OPTIMIZATION WITH COILSIM1D

Alexander Vervust

*Laboratory for Chemical Technology
Ghent University*

Ismaël Amghizar

*Laboratory for Chemical Technology
Ghent University*

Andrés E. Muñoz G.

*R&D Manager
AVGI*

Kevin M. Van Geem

*Laboratory for Chemical Technology
Ghent University*

Guy B. Marin

*Laboratory for Chemical Technology
Ghent University*

Prepared for Presentation at the 2016 Spring National Meeting
Houston, Texas, April, 13, 2016

AICHE and EPC shall not be responsible for statements or opinions contained in papers or printed in its publications

FULL FURNACE SIMULATIONS AND OPTIMIZATION WITH COILSIM1D

Alexander Vervust

Laboratory for Chemical Technology

Ghent University

Ismaël Amghizar

Laboratory for Chemical Technology

Ghent University

Andrés E. Muñoz G.

R&D Manager

AVGI

Kevin M. Van Geem

Laboratory for Chemical Technology

Ghent University

Guy B. Marin

Laboratory for Chemical Technology

Ghent University

Abstract: COILSIM1D is a steam cracking simulation package that has been developed as the result of several decades of independent research and modelling activities at the Laboratory for Chemical Technology (LCT) of Ghent University. Using a friendly graphical user interface, it combines a detailed fundamental kinetic model with a one-dimensional reactor model, which provides high flexibility regarding reactor geometries, feeds and simulation strategies. Simulations for a very broad range of complex feeds up to (hydrotreated) VGO can be easily performed thanks to SIMCO, a molecular reconstruction module incorporated in the software based on commercial indices of the feed. Over time, and based on own and client initiatives, various other features have been incorporated into COILSIM1D, such as TLE and run length simulations, or a shooting method that allows to perform simulations using a variety of severity indicators as boundary conditions at the reactor outlet. Recently, the kinetic model has been expanded and fine-tuned based on data from a large ethylene producer, including oxygenates; a firebox and convection section model has been incorporated, to allow full cracker simulations (i.e. convection, firebox, reactor and TLE altogether) in a unique package, and with short simulation times. COILSIM1D has also been linked with Aspen and other process simulators. Illustrative simulations have been carried out to show the operation of these new features, which effectively take COILSIM1D to a new level, transforming it into a whole-furnace simulation and optimization package.

Introduction

COILSIM1D is a comprehensive steam cracking simulation package, developed as the natural result of several decades of independent research and modelling by the Laboratory for Chemical Technology (LCT) of Ghent University. AVGI, a spin-off company from Ghent University, recently acquired all technical and commercial rights to COILSIM1D. With this, further and faster development of the software can be carried out, whilst interacting on a business-to-business structure with clients spread over four continents, allowing for customization of the package, tailored to the specific needs of the client.

The first two AVGI-driven developments of COILSIM1D have been carried out within a framework of collaborative work with LCT, and comprise the expansion and fine-tuning of the kinetic network used to describe the chemistry of the process, as well as the incorporation of furnace simulation capabilities that allow users to carry out full cracker simulations in one software package, with an even higher level of accuracy at the reactor level.

COILSIM1D has been traditionally developed as a reactor simulator aimed at the prediction of yields at the reactor outlet, combining a fundamental single-event kinetic network with a one-dimensional plug-flow reactor model. Over time, and based on own insights and permanent interaction with the increasing number of licensees, new functionalities have been gradually added to the package, that are made available to all clients having annually renewable license agreements by means of regular updates. Clients using evaluation licenses also receive the most updated version of COILSIM1D.

All these functionalities have conferred large flexibility to COILSIM1D, making it able to handle a very broad range of reactor geometries, feeds and operating conditions. A feedstock reconstruction method (SIMCO) is integrated in the package, which allows to reconstruct the molecular composition of light mixtures to HVGO feeds, based on simple and easily available commercial indices of the feed. Also a module to carry out TLE simulations is incorporated, allowing to account for the effect of this equipment on the process yields, effluent temperature, and heat recovery.

Different simulation approaches can be applied with COILSIM1D, depending on the information that the user has available: heat-flux or temperature profiles along the reactor can be defined; outlet conditions based on frequently used severity indices can also be specified, such as the Coil Outlet Temperature (COT), the conversion of a given species, the ratio of propylene to ethylene in the effluent (P/E), or that of methane to propylene (M/P). Additionally, dedicated routines for yield maximization, sensitivity analysis and run length estimation are incorporated in COILSIM1D, enabling users to straightforwardly optimize their process while taking multiple targets into account.

Following the market's urge to count on a single tool that is able to accurately simulate steam crackers as a unit (i.e. firebox, convection section, reactor and TLE in one package), AVGI and LCT took on the challenge of taking COILSIM1D to the next level, successfully transforming it into a whole cracker simulation package.

This paper presents an overview of the main features of COILSIM1D, paying particular attention to the most recent developments regarding the kinetic network, as well as the firebox and convection section models. To demonstrate the operation of these new features and their

harmonious integration in the already existing package, illustrative simulations combining the new and already existing models are presented. The user-friendliness of COILSIM1D and its ability to easily interact with external software packages are also discussed.

The COILSIM1D Simulation Package

SIMCO: Feedstock Reconstruction from Common Commercial Indices

To be able to take advantage of the flexibility and accuracy that a fundamental kinetic model can offer, knowledge of the detailed molecular composition of the used feed is crucial and will affect the accuracy of the obtained simulation results.¹ For liquid fractions, which can be made up of several thousands of different components, detailed feedstock compositions are not straightforward to determine; not even for naphtha fractions. Existing analytical state-of-the-art techniques such as GCxGC, can be used to determine the detailed feedstock composition, but they are costly and can be very time consuming. In industry, feed composition can change significantly on a daily or even hourly basis and hence these analyses are not feasible to perform.

A feasible alternative are feedstock reconstruction methods, that allow to compute a detailed molecular composition of the feedstock based on common commercial indices, e.g. the average molecular weight, information regarding boiling points, the specific density, the global PIONA weight fractions, etc. The ease to reconstruct different feeds makes SIMCO a powerful tool for rapid and accurate feed reconstruction. This numerical tool comes with a user friendly GUI, depicted in Figure 1, in which the different input parameters are filled in by the user in the units of choice.

Boiling Point (%)	Value
IBP	-10.3
5%	32.37
10%	58.63
20%	62.99
30%	86.99
40%	100.88
50%	117.8
60%	127.96
70%	152.76
80%	178.83
90%	230.06
95%	295.13
FBP	337.23

Figure 1: The GUI of SIMCO, where different parameters can be filled in as input for reconstruction of a feed.

Commercial indices can be determined by means of relatively fast and low cost standardized analytical procedures. In this respect, SIMCO, the feedstock reconstruction method available within the COILSIM1D package, is a powerful tool for industry to simulate the complex molecular composition as input for a fundamental kinetic model. SIMCO uses two methodologies, one based on the Maximisation of the Shannon Entropy (MSE)^{2,3}, and another based on an artificial

neural network (ANN).⁴ MSE is the most general method and can be used for virtually every hydrocarbon feed. ANN, on the other hand, has shown to be more accurate for naphthas, provided that their characteristics fall within the application range of the network's training set.⁴ The most suited method to reconstruct the feedstock is automatically selected by the software, offering the highest reliability on the reconstructed feed and the subsequent simulated product spectra. This enables users to take optimal advantage of feedstock flexibility. The feed reconstruction method also incorporates sulfur components. The reconstructed feed can be directly imported into a reactor simulation.

Reactor Definition

COILSIM1D incorporates an extensive built-in library that includes the reactor configurations most commonly used in industrial steam crackers. In this way only the length, internal diameter and wall thickness of each section have to be provided as input by the user. Since the reactor model of COILSIM1D can be applied to any type of tubular reactor, virtually any other reactor geometry that is not included in the built-in library can be easily implemented using the 'New coil geometry' tool in the GUI, as shown in Figure 2. The user can also choose from an assortment of reactor materials. Fins or other 3D geometries (e.g. straight, riffled, spiral) are also supported and accounted for. User defined reactor geometries can be saved and reused later in future simulations.

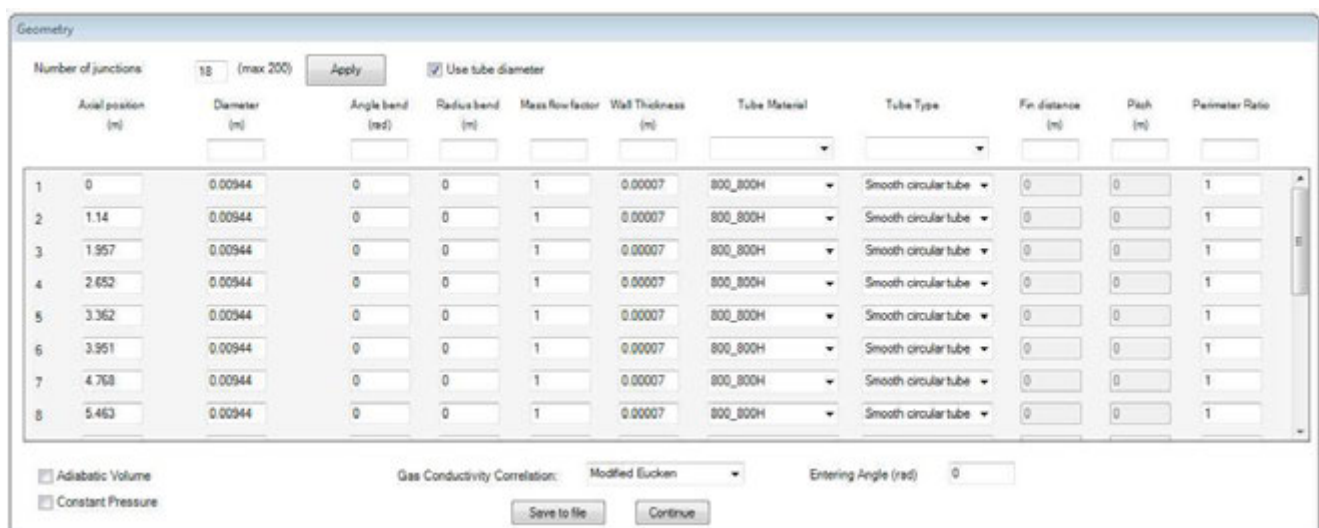


Figure 2. New coil geometry tool included in the GUI of COILSIM1D.

Transfer Line Exchanger

To explicitly account for the effect of the rapid quenching of the process gas leaving the reactor, COILSIM1D incorporates a TLE simulation model.⁵ It takes into account the heat transfer from the process gas side to the steam/water mixture used for cooling. The high heat content of the process gas is usually used to produce high pressure steam and hence accurate simulations of this element are highly important for integral simulations of the furnace as a whole.

Different simulation strategies are possible with COILSIM1D, using either a specific water mass flow rate or a specific steam quality as boundary conditions. The model also allows the simulation of a full thermosiphon, which can be used to estimate the water recirculation rate as well as the steam production.

The TLE model is designed specifically to simulate double piped TLEs, like the one shown in Figure 3, which are the most common configuration in current commercial furnaces. In this type of TLE, the cracked gas flows through the inner tube and the water/steam mixture flows through the outer tube. Since the temperature of the cracked gas is still considerably high, the secondary reactions that can take place in the inner tube of the TLE are explicitly accounted for.

This module also includes a dedicated model to account for fouling in the TLE, caused mainly by the condensation of the heavy hydrocarbons that are often present in the reactor effluent. ⁶⁻⁸ Combined with the coke deposition models for gaseous and liquid feeds used in the reactor section, this feature provides the user with a very handy tool for the estimation of run lengths.

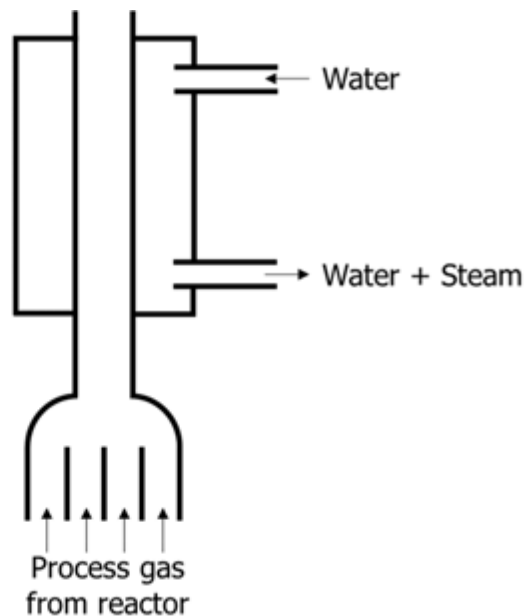


Figure 3. Schematic of a double piped TLE used to quench the effluent of reactor coils.

Run Length Simulations

Steam cracking is inevitably associated with the deposition of coke on the inner wall of the reactor, which largely affects the economics of the process. ⁹ Since decoking operations translate into loss of production capacity, accurate prediction of the run length of a furnace is highly interesting for the optimization of cracking furnaces. COILSIM1D offers the possibility to perform run length simulations that account for the effect of coke depositing inside the reactor over the course of a run, until the operational limitations are reached.

To accurately predict the formation of coke, two different models are incorporated: one for gaseous feeds ¹⁰ and one for liquid feeds ¹¹. Both account for the heterogeneous non-catalytic or so-called asymptotic coking regime, which is dominant over most of the run length. ^{12, 13} The

effect of the brief catalytic coking regime can be accounted for in COILSIM1D, by giving the model an estimate of the expected duration of the catalytic coking regime.

The coking rate is computed using the selected model, and the increase in coke thickness during each specific time step is calculated and added to the already deposited layer, until reaching the maximum TMT or maximum pressure drop, as defined by the user in the GUI. An illustrative example of simulation results is shown in Figure 4, where the calculated TMT (accounting for faster catalytic coking at the beginning of the run) is plotted as a function of time. It is clear that the slope of the TMT rapidly drops to a constant value as a consequence of the shift of the dominant coke deposition mechanism.

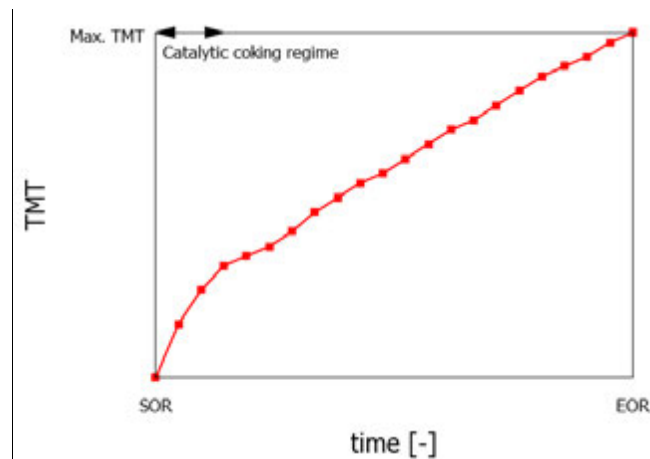


Figure 4: TMT as a function of time for a simulation case that accounts for a faster catalytic coking regime at the beginning of the run.

New Features of COILSIM1D

Kinetic Model for Steam Cracking of Hydrocarbons

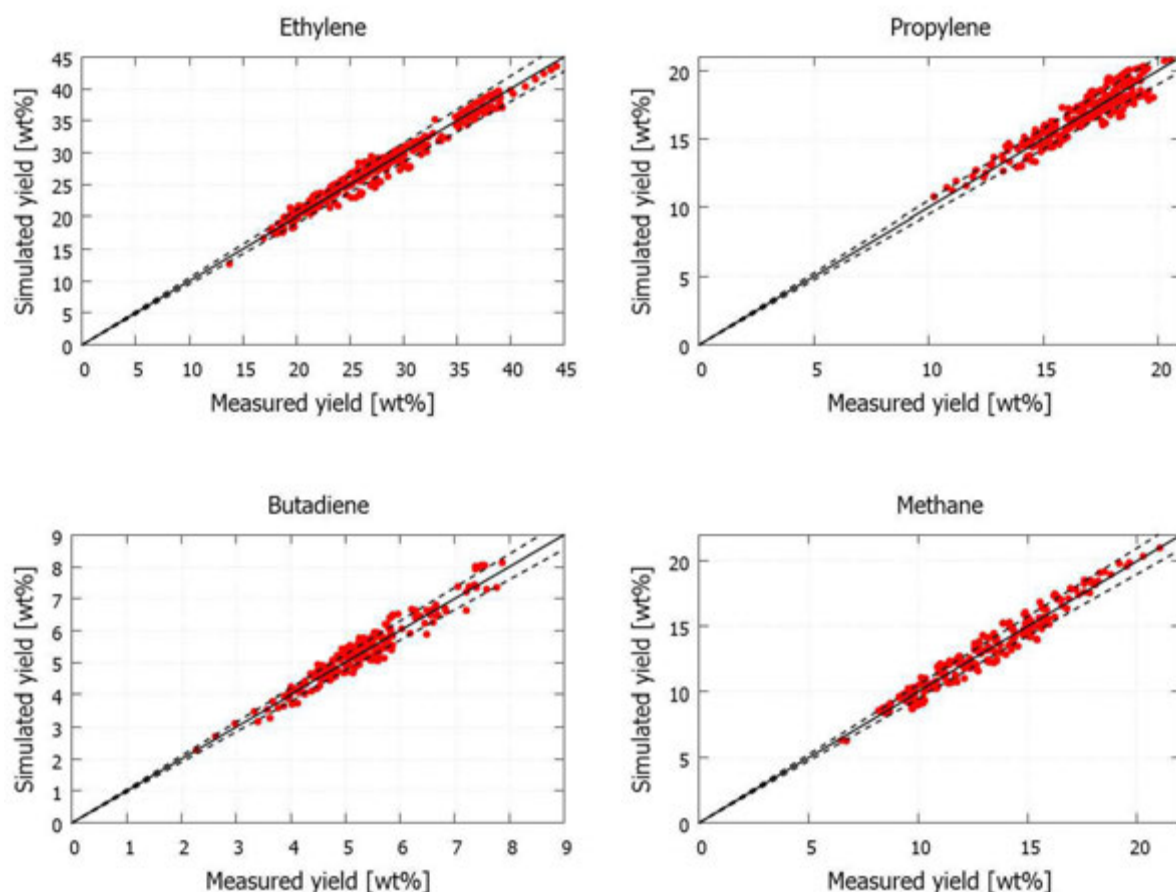
The kinetic model of COILSIM1D is assuredly the most important feature of this software package. COILSIM1D comprises a very thorough mathematical model that consists of two parts: (i) A single event kinetic model called CRACKSIM,¹ which accurately describes the chemistry taking place in the reactor; and (ii) a one dimensional tubular reactor model describing the transport phenomena. The model equations are valid for any type of tubular reactor, allowing COILSIM1D to be used for a broad range of coil configurations. Both parts complement each other and help to structure a mathematical description of the problem to simulate. A dedicated fast and robust solving algorithm is applied to solve the mathematical problem. The required simulation time is usually less than 1 second allowing to simulate within a broad window of conditions and feeds in a limited time.

The accuracy and robustness that are characteristic of CRACKSIM are, to a great extent, the result of the fundamental approach that it uses, i.e. describing each of the occurring reactions as a single step, instead of simply accounting for global reactions. The corresponding

kinetic and thermodynamic parameters are calculated using consistent and dedicated high level ab-initio calculations.¹⁴⁻¹⁹ It is therefore no surprise that COILSIM1D incorporates the broadest and most accurate reaction network for steam cracking of hydrocarbons.

The kinetic model has been recently extended, to incorporate also common oxygenate contaminant species whose thermochemical decomposition yields products such as methanol and aldehydes, known for leading to several downstream process difficulties such as gum formation and off-spec products.

Currently more than 720 different molecular species and 43 radical species are incorporated, leading to a global network of more than 300,000 reactions. The model has been validated using an extensive set of data points originating from industrial furnaces, as well from the pilot plant and bench scale set steam cracking setups of LCT. The validation dataset includes a broad assortment of feeds, ranging from ethane to complex and heavy mixtures such as gasoil, waxes and even crude oil. Excellent agreement is observed between the measured and predicted yields of the main and minor products,^{1, 20} as shown in the parity plots presented in Figure 5.



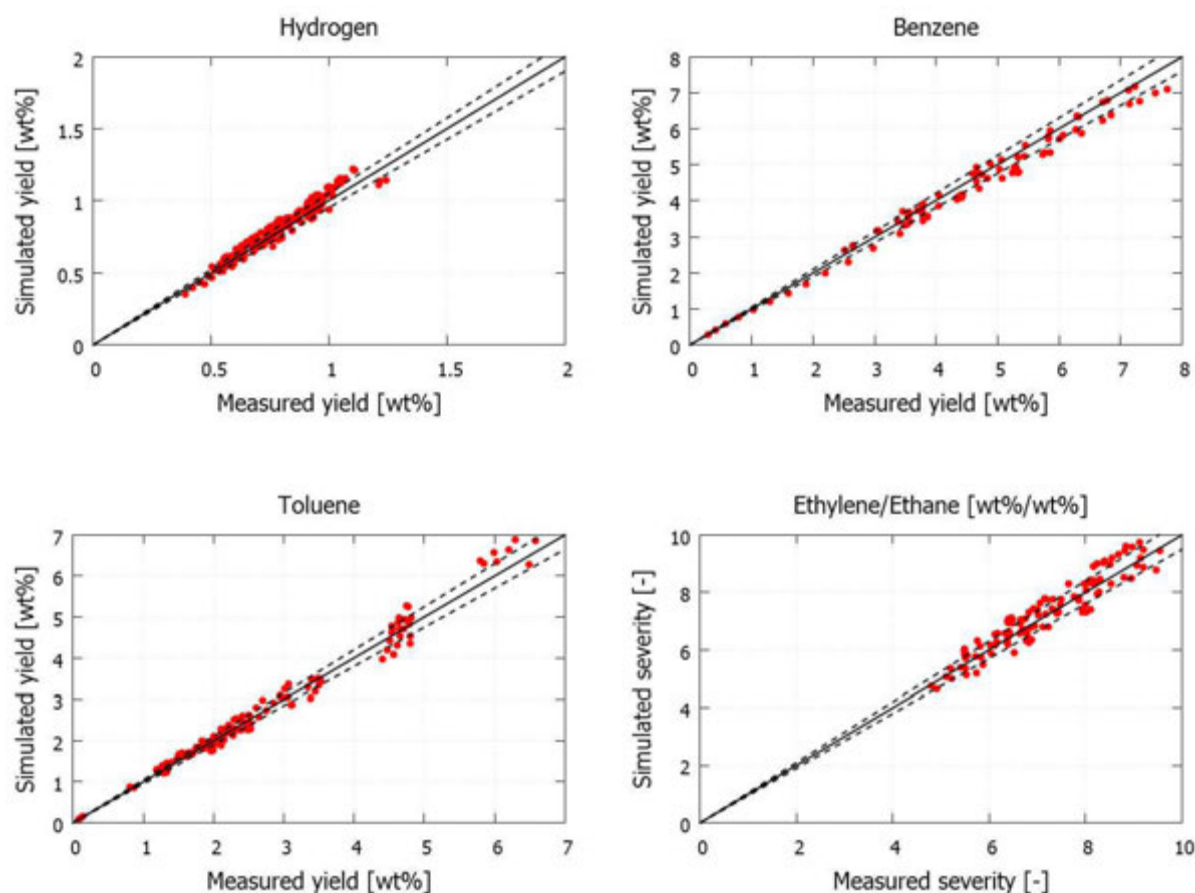


Figure 5: Parity plots comparing measured and simulated yields of various cracking products. Dashed lines indicate $\pm 5\%$ deviations.

Convection Section

The convection section is a new feature of COILSIM1D, and it is part of the furnace module of the GUI, which comprises two complementary models for simulations of firebox and convection section. The convection section simulations help to estimate different process parameters of interest such as flue gas temperature, utility steam production and total thermal power exchange based on limited user input.

When feeding liquids, evaporation also takes place in the convection section, which is an important aspect to consider for design and optimization, especially when dealing with heavy feeds that might not be completely evaporated and thus lead to fouling, in particular in the lower banks. Explicitly taking evaporation into account can help to locate hot spots and hence prevent extensive fouling of the convection banks. To meet this challenge, a dedicated equilibrium based evaporation model has been developed.

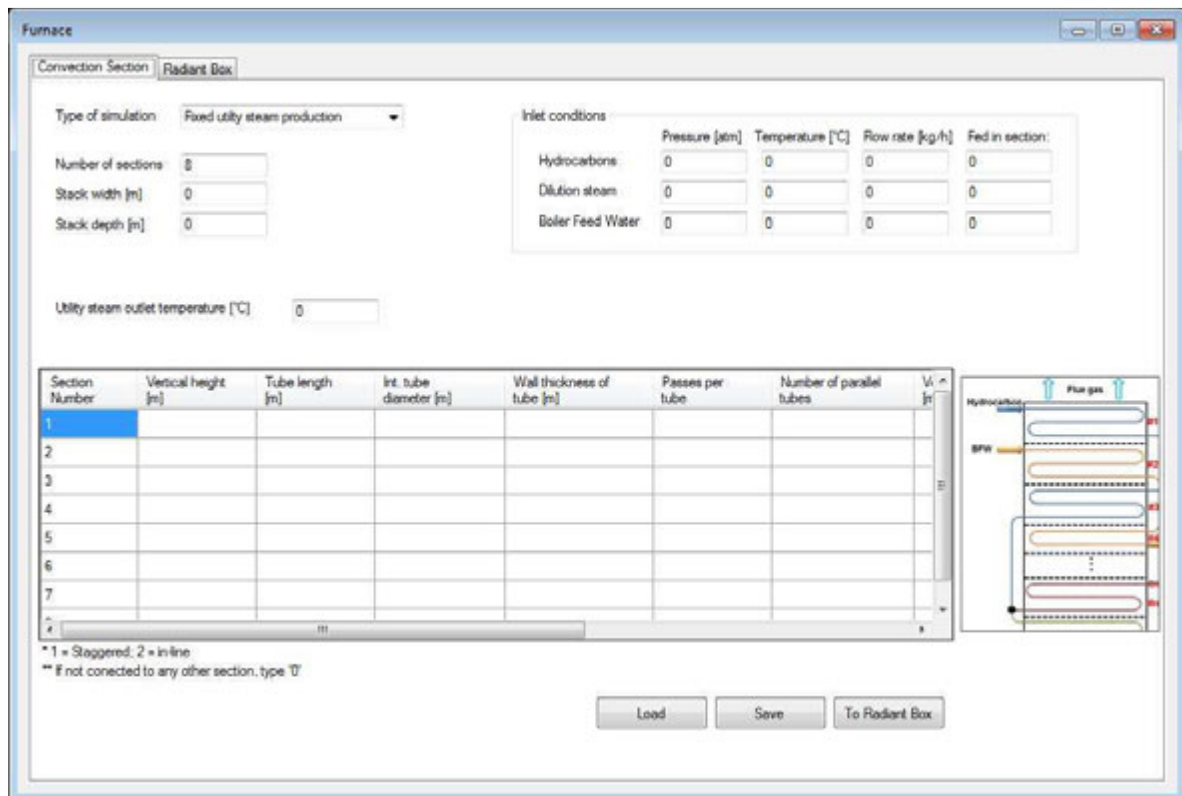


Figure 6: GUI of the convection section simulation module of COILSIM1D.

The convection section is modelled as a finite number of tube banks in-series. As can be seen in Figure 6, the user can define the number of banks and the number of parallel tubes on each bank, which can make multiple passes. The feed entering each bank can be either a stream entering the convection section for the first time, a stream originating from another bank, or a mixture thereof. Furthermore, different tube arrangements (in-line or staggered) are supported, as well as different configurations (counter and concurrent flow), as shown in Figure 7. Additionally, different tube materials, with characteristic roughness and thermal properties can be chosen. The model can also account for the usage of finned tubes. In this way, virtually any type of convection section configuration can be easily simulated with COILSIM1D.

The model describes the duty pick-up of each bank from the hot flue gas to the process stream, based on different user input and process conditions (e.g. throughputs, composition, temperatures), parameters from the firebox (thermal efficiency, combustion fuel rate, bridge wall temperature) and TLE (heat duty, steam flow rate). The tool contains an extensive library of pressure- and temperature-dependent physical properties for all the molecular species available in COILSIM1D.

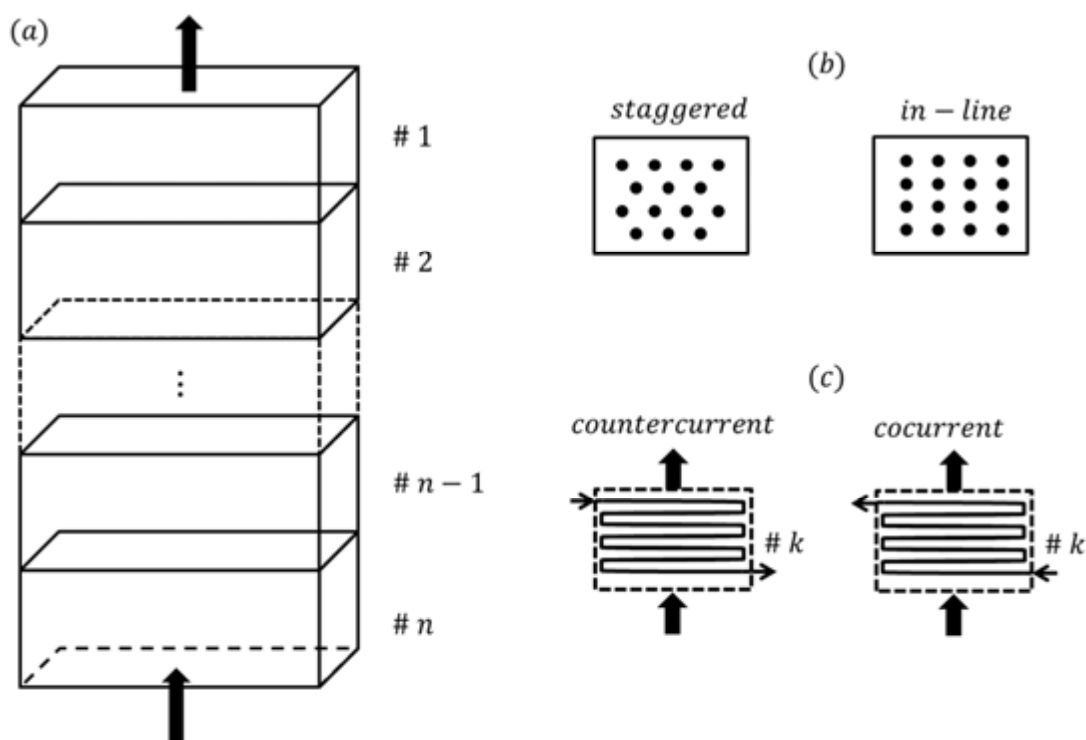


Figure 7. Schematic representation of the convection section in COILSIM1D: (a) tube banks in series; (b) supported tube arrangements; (c) supported flow pattern arrangements.

To illustrate the use of the convection section module, a demonstration case has been simulated for a typical arrangement, presented in Figure 8. The geometry of the convection section (i.e. number of passes, tube lengths, number of parallel tubes and pitch lengths) was defined via the GUI, as well as the mass flows of the input streams and the number of the bank in which they enter the convection section. Eight heat exchanging tube banks and six different inlet streams are defined. The naphtha is fed to the first bank, then mixed with dilution steam and taken to the third bank. The mixture is further heated in banks 3 and 4. The heated mixture is then mixed with superheated dilution steam (outlet stream from bank 7), and conducted to the lowest bank. The second bank is used to heat water at high pressure. High pressure steam is overheated in bank 5 and then mixed with desuperheating water. The resulting stream is then heated up in bank 6.

The hydrocarbon feed was reconstructed using SIMCO, based on a set of common commercial indices presented in Table 1. The reconstructed naphtha consists of 72 different components ranging from C₄ to C₁₁.

The calculated Coil Inlet Temperature (CIT) is 578.3°C and the pressure before the Venturi nozzles is 3.8 bara. These values are typical for a naphtha cracker,²¹ and can be subsequently used as input for the reactor model to determine the product distribution.

Table 1. Commercial indices used for reconstructing the naphtha feed with SIMCO

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

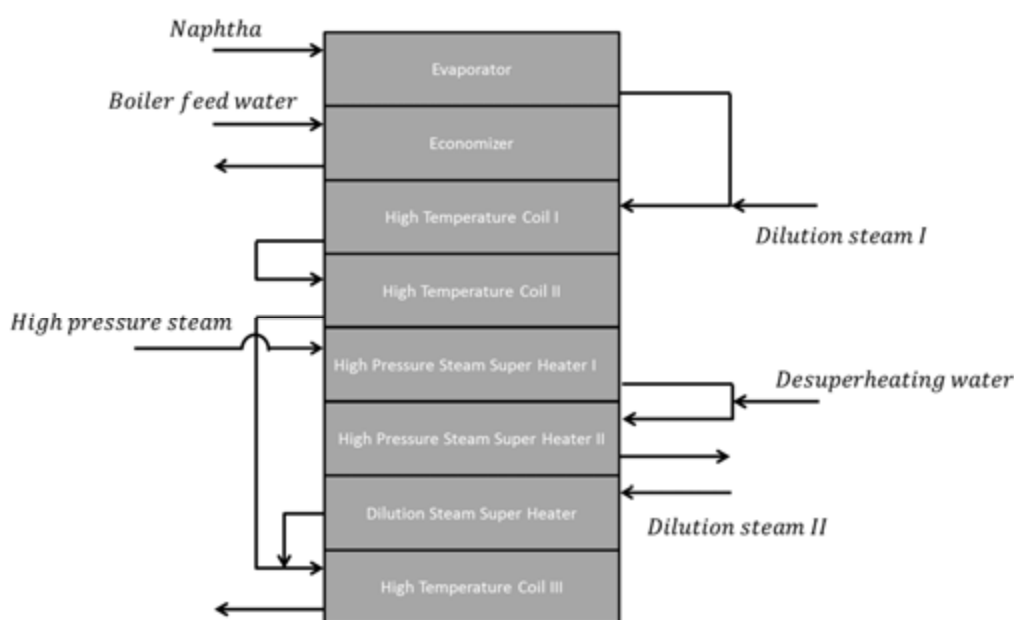


Figure 8. Schematic representation of the simulated convection section.

The calculated temperature profiles of the flue gas and process streams are shown in Figure 9. The flue gas leaves the stack at a temperature of 283°C, whilst the bridge wall temperature is estimated to be 1195°C. The vapor fraction is estimated to be 98.39% at a temperature of 301.4°C, indicating that the feed is almost completely evaporated in the first bank. It is worth noticing that, according to the ASTM D86 boiling points given in Table 1, the feed should be completely evaporated at such a high temperature, but due to the substantially high pressure in the evaporator (6 bar), the boiling points of the species are significantly higher than under atmospheric pressure. This shows the importance of accounting for pressure dependence when simulating the phase transition from liquid to vapor.

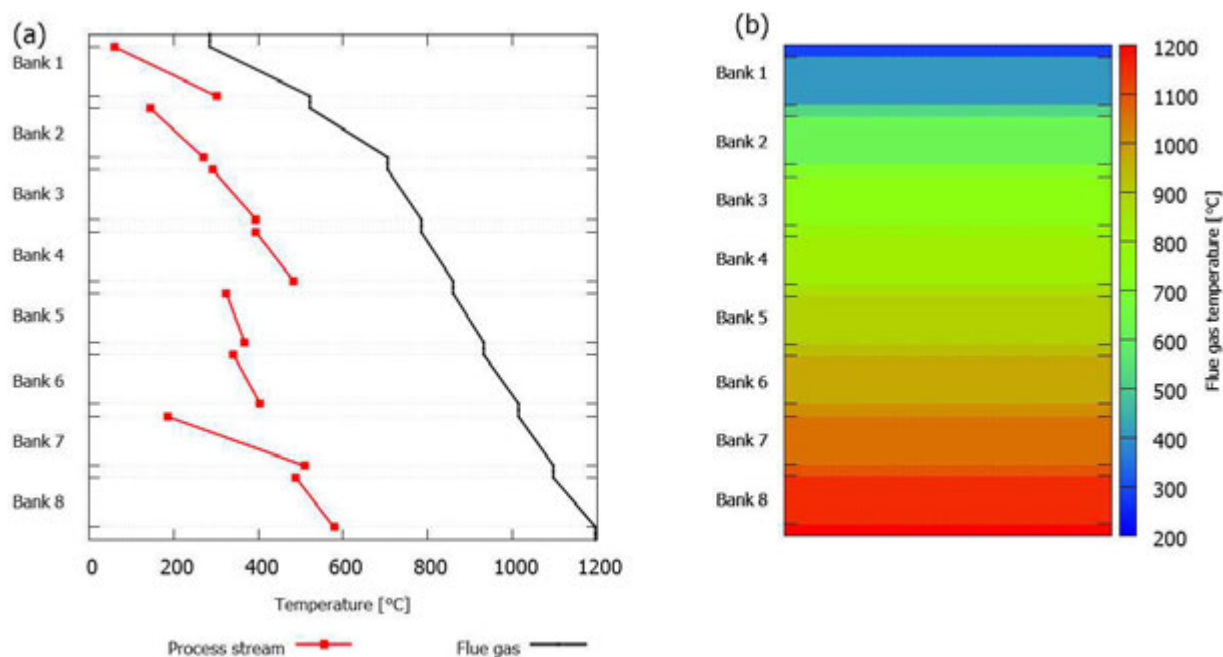


Figure 9. (a) Temperature profile of the process streams for all banks, (b) flue gas temperature profile along the convection section

Firebox Simulation Model

With the implementation of a firebox model, COILSIM1D is able to estimate additional process parameters of interest, such as the flue gas temperature profile inside the firebox, the bridge-wall temperature, the furnace efficiency and the heat flux profile to the reactor coils. Using the GUI of COILSIM1D, shown in Figure 10, the user can easily provide the geometry and operating conditions of the firebox, required as input for the simulation. The user is able to specify the furnace geometry, the type of burners (i.e. floor and/or wall burners) and, in the case of wall burners, the heights at which they are located. Also the operating conditions, such as the inlet temperatures and mass flow rates of fuel and oxidizer (e.g. air) per burner, and the operating pressure, are to be specified. This flexibility in user input guarantees the applicability of the model for a broad range of cracking furnaces.

The firebox model has been coupled to the reactor model, enabling the estimation of process yields, COT, COP, etc. of cracking furnaces, based on the geometry and inlet conditions of the furnace and tubular reactors, specified by the user.

An illustrative simulation of the firebox, reactor and TLE has been carried out with COILSIM1D for a Kellogg Millisecond furnace, shown in Figure 11 (left). The dimensions and operating conditions of the reactor and TLE are presented in Table 2. The simulation parameters are straightforwardly input by means of the GUI of COILSIM1D, as illustrated in Figure 10 for the geometry and operating conditions of the firebox. 53.9 kg/h of fuel ($\text{CH}_4 + 5\% \text{H}_2$) are supplied to each long flame burner and burnt using air at ambient conditions. The software converts the three-dimensional furnace dimensions to their one-dimensional equivalent and discretizes the furnace along its height, as illustrated by the dotted lines in Figure 11 (right).

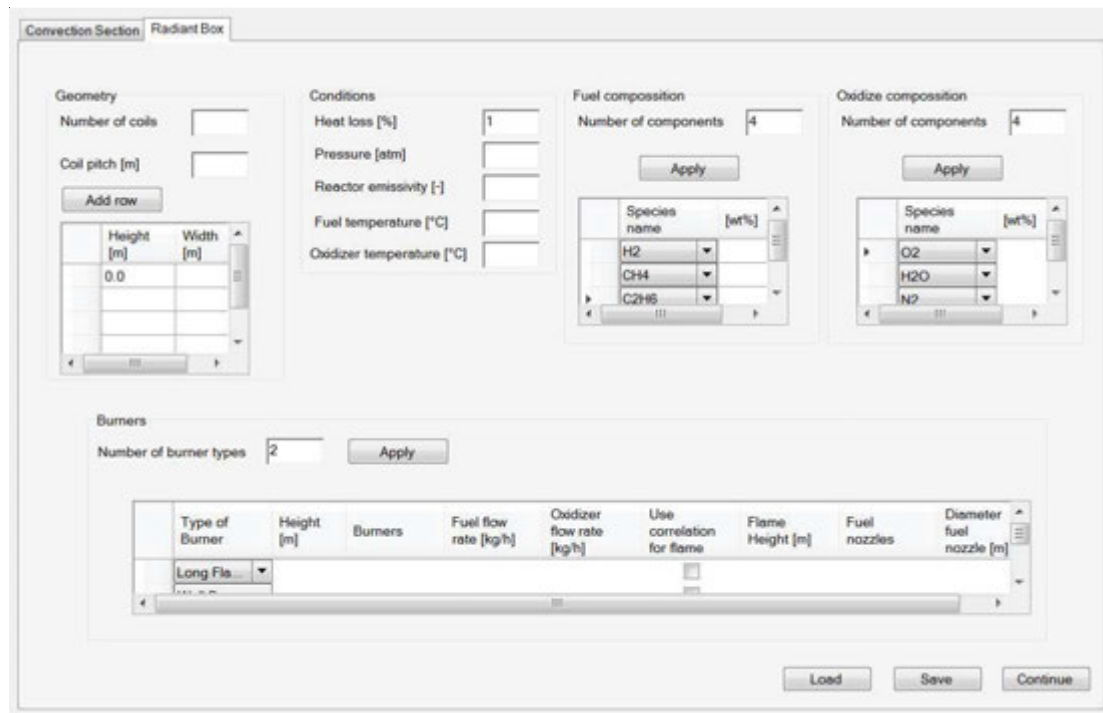


Figure 10. GUI of the firebox simulation module of COILISM1D.

Table 2. Dimensions and operating conditions of the reactor and TLE of the Kellogg Millisecond furnace

Reactor dimensions		Feed composition [wt%]	
Length [m]	10.556	C ₃ H ₈	92.25
Internal diameter [m]	0.0348	C ₂ H ₆	1.05
		C ₃ H ₆	3.02
Operating conditions		i-C ₄ H ₈	0.33
Feed mass flow rate [kg/h]	118.5	1-C ₄ H ₈	0.27
Steam dilution [kg/kg]	0.3265	2-C ₄ H ₈	0.08
Coil inlet temperature [°C]	630.5	i-C ₄ H ₁₀	1.93
Coil inlet pressure [bara]	2.35	n-C ₄ H ₁₀	0.45
		C ₅ ⁺	0.62
TLE dimensions			
Length [m]	9.369		
Diameter inner tube [m]	0.067		
Diameter outer tube [m]	0.119		
Number of joining coils [-]	4		

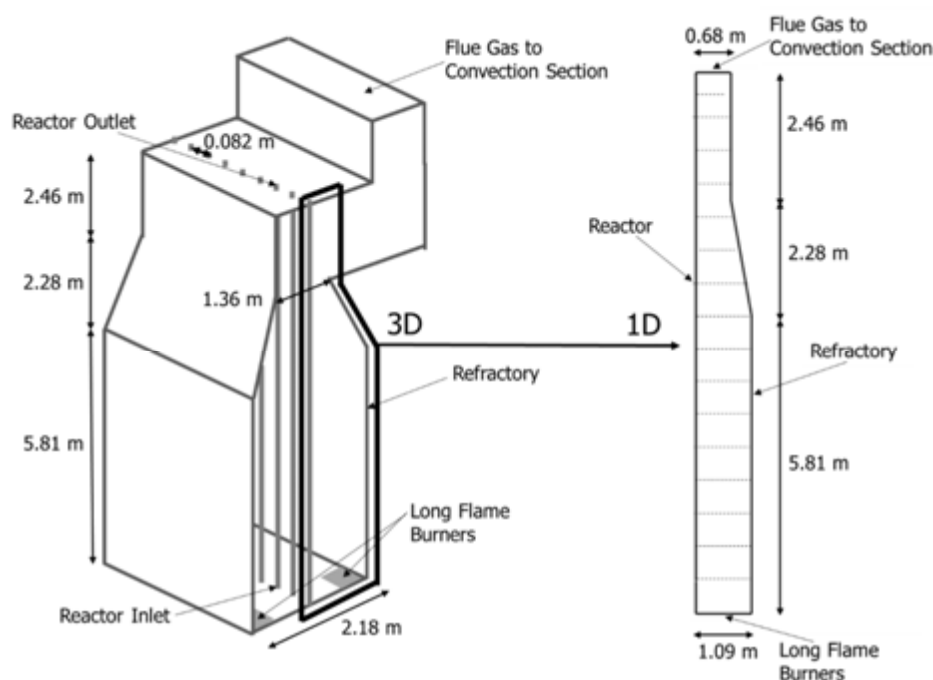


Figure 11. Three-dimensional geometry of the radiant section of a Kellogg Millisecond furnace (left) and its equivalent one-dimensional geometry used for the COILSIM1D simulation (right).

Table 3 shows the results of the COILSIM1D simulation, together with industrially measured values. The simulated values agree well with the available industrial data. The simulation results demonstrate not only the accuracy with which COILSIM1D predicts the process yields, but also its ability to estimate other parameters, such as the COT, furnace efficiency and bridge-wall temperature. Since the GUI facilitates setting up the simulation and considering that the computational time is less than one minute on one core of an Intel® Core™ i7-5600U CPU @ 2.60 GHz processor, this simulation case illustrates the ease and speed with which steam crackers can be simulated using COILSIM1D.

Table 3. COILSIM1D-simulated and industrial ²² data for the Kellogg Millisecond furnace.

	Simulated	Industrial*
Product Yields [wt%]		
H ₂	1.5	1.6
CH ₄	19.9	19.3
C ₂ H ₂	0.7	0.8
C ₂ H ₄	35.1	35.1
C ₂ H ₆	2.7	2.9
C ₃ H ₄ (MA)	0.3	
C ₃ H ₄ (PD)	0.1	0.7
C ₃ H ₆	17.0	17.0
C ₃ H ₈	15.8	15.7
1,3-C ₄ H ₆	1.8	1.9
1-C ₄ H ₈	0.8	1.2

2-C ₄ H ₈	0.4	
i-C ₄ H ₈	0.3	0.2
i-C ₄ H ₁₀	0.2	0.1
n-C ₄ H ₁₀	0.1	0.1
Other properties		
Reactor coil outlet temperature [°C]	878.9	
Temperature at exit TLE [°C]	445.9	435
Furnace efficiency [%]	43.2	
Bridge-wall temperature [°C]	1138	

*Industrial data are measured downstream from the transfer line exchanger (TLE).

Input/Results Files and Interaction with External Software

COILSIM1D is a text-based simulation tool. The user friendly GUI allows the user to easily set up a simulation case step by step. Operating parameters (and their units), simulation strategies and geometrical input can be typed in manually by the user, or can be loaded from previous simulation cases.

```

0      'fraction type(0,1,2,3 or 4)'
0      'reconstruction method (0,1 or 2)'
0.00   'Average molecular weight (g/mol)'
0.00   'H/C ration (kg/kg)'
0.7088 'density (60 ° F) (g/ml)'
0      'Mass/volume indicator (0 or 1)'
0      '0:PIONA, 1:PNA, 2:SA'
36.50  'Total amount of paraffins (wt% or vol%)'
32.80  'Total amount of isoparaffins (wt% or vol%)'
0.00   'Total amount of olefins (wt% or vol%)'
21.40  'Total amount of naphthenes (wt% or vol%)'
9.20   'Total amount of aromatics (wt% or vol%)'
0      'boiling point unit (0,1 or 2)'
0      'boiling point curve type (0,1 or 2)'
39.00  'initial boiling point (' C,K or 'F)'
0.00   '5% volume boiling point (' C,K or 'F)'
0.00   '10% volume boiling point (' C,K or 'F)'
0.00   '20% volume boiling point (' C,K or 'F)'
0.00   '30% volume boiling point (' C,K or 'F)'
0.00   '40% volume boiling point (' C,K or 'F)'
99.00  '50% volume boiling point (' C,K or 'F)'
0.00   '60% volume boiling point (' C,K or 'F)'
0.00   '70% volume boiling point (' C,K or 'F)'
0.00   '80% volume boiling point (' C,K or 'F)'
0.00   '90% volume boiling point (' C,K or 'F)'
0.00   '95% volume boiling point (' C,K or 'F)'
165.50 'final boiling point (' C,K or 'F)'
0      'NMR H (arom) (%)'
0      'NMR H alpha (%)'
0      'NMR H beta (%)'

```

Figure 12: Example of an input file used for feedstock reconstruction with SIMCO.

All the input values are then used to create well-organized input files that are stored into project folders specifically created for each simulation. These input files are simple, self-explanatory, and have a fixed format. An example of an input file used for feedstock reconstruction is shown in Figure 12. The user manual of COILSIM1D explains the purpose and structure of all the input and output files.

The GUI incorporates a tool for quick visualization of the main results of a simulation, as shown in Figure 13. Furthermore, the GUI also displays the results (yields, temperatures, ...) in the form of graphs, which facilitates interpretation of the simulated results. This feature is illustrated in Figure 14. The files with all the simulation results are also stored in the project folder, and can be imported into spreadsheets for further analysis or post-processing.

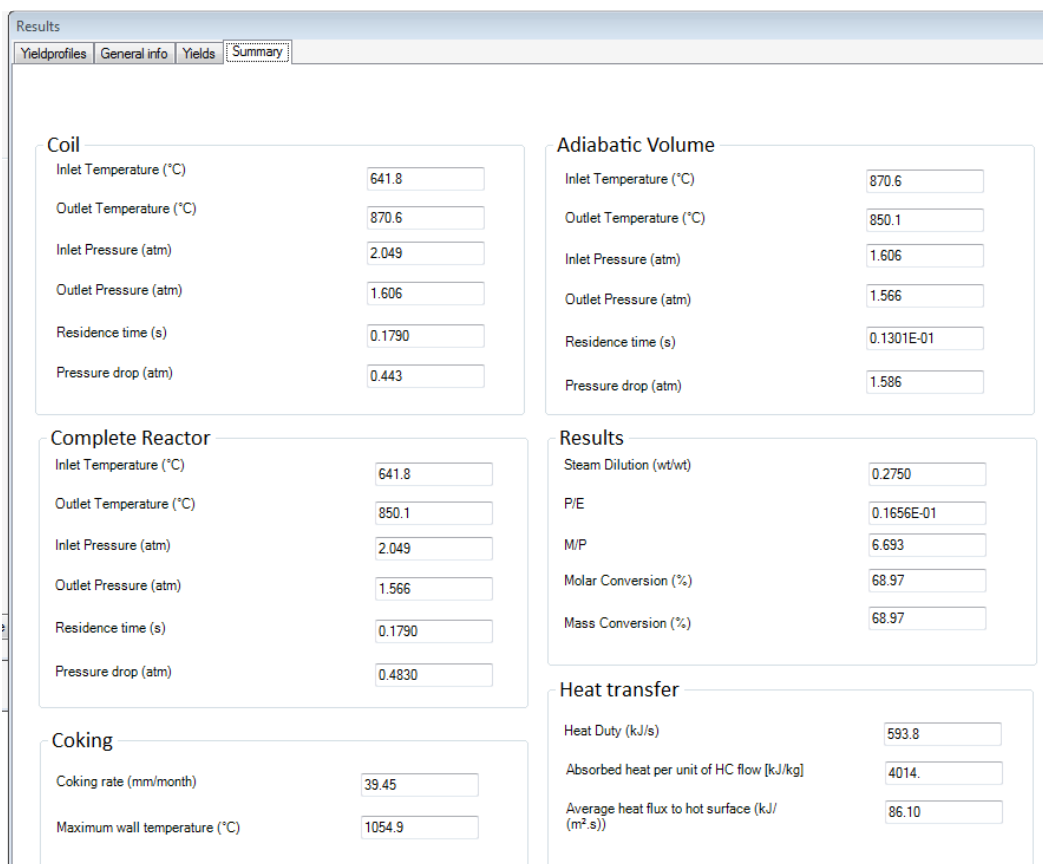


Figure 13: Results tab of the GUI, showing the main results of a simulation

Since the input/output files have a fixed format, they can be easily created and modified without using the GUI, thus allowing users to make use of scripts in the programming language of their preference to take care of these tasks. COILSIM1D includes also an executable file, which allows to carry out simulations bypassing the GUI. This enables users to write scripts for automated creation and execution of large batches of simulations without the need of constant human input.

The ability of COILSIM1D to work using text input/output files has the additional benefit of enabling easy interaction with external software packages, e.g. Aspen Plus®, HYSYS® or gPROMS. This way, whole plant simulations can be made taking into account the constraints of all the units involved. The interaction is simple and based on an interfacing script that reversibly converts the species and process conditions representation of both software tools. Integration with unit operation software packages or in-house optimization tools has been successfully performed with several licensees, considering their specific requirements. Integration of COILSIM1D in real time optimization has also been successfully carried out in a demonstration unit in Asia, showing great potential for industrial scale implementation.

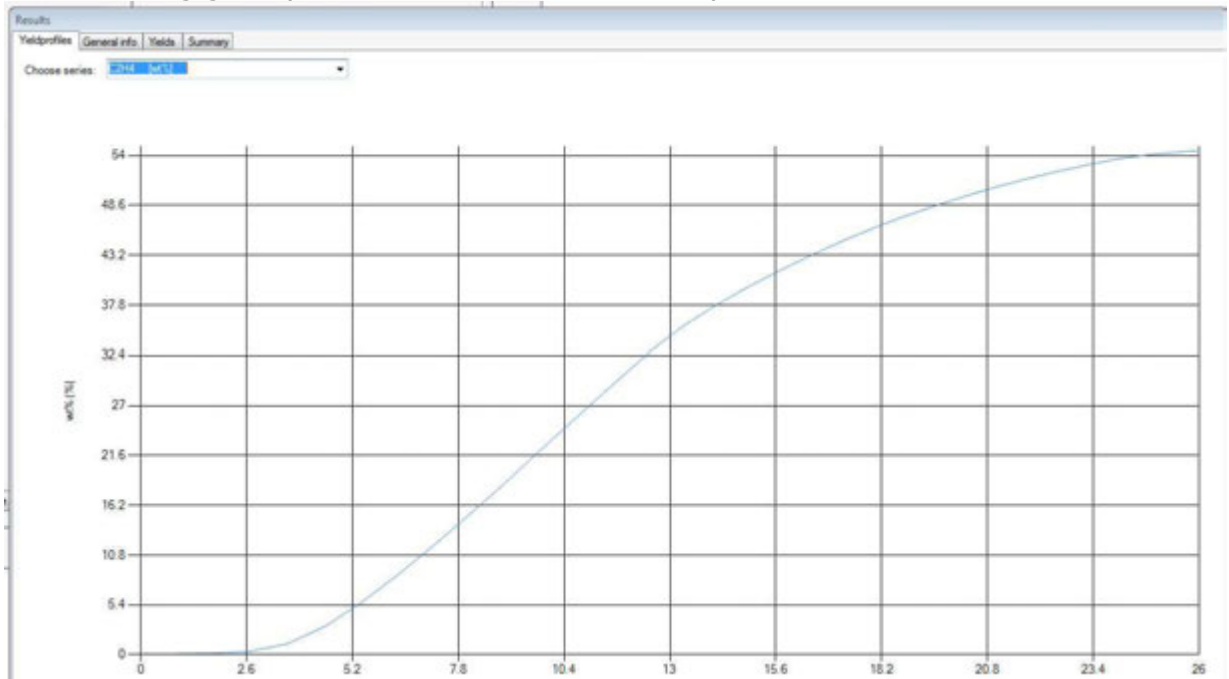


Figure 14: Graphic representation of yield profiles in COILSIM1D

Conclusions

COILSIM1D is a comprehensive simulation package for steam cracking processes. Its main strength lies in its fundamental kinetic model, the broadest currently available. Various features and simulation strategies have been developed and implemented in COILSIM1D: SIMCO, a molecular feedstock reconstruction method; a module to simulate the TLE; a module to estimate reactor run lengths using dedicated coking models; and a shooting method, that allows to carry out simulations using severity-related indices as boundary conditions. To take COILSIM1D to the next level and transform it into a whole furnace simulation package, new features have been incorporated and the kinetic model has been fine-tuned and further extended to account for oxygenate species.

A model to simulate the convection section of a steam cracker has been developed. It allows the user to evaluate the impact of a broad range of different process conditions and feeds in the process. Despite requiring a limited amount of input data, this model helps to easily evaluate the effect of a broad range of different process conditions and feeds. This is a very helpful tool for design and optimization of new and existing configurations. The model accurately accounts for the evaporation of the feed and can be used to prevent fouling in the convection section, which has significant technologic and economic impact on the process. An example simulation was defined and executed yielding satisfactory results.

Another new feature is the firebox model, which allows to reliably determine heat flux profiles for the reactor, and various other parameters of interest, such as the bridge wall temperature and thermal efficiencies. The model can be applied to a variety of firebox geometries, burner arrangements and fuel compositions. It has been successfully used to simulate a propane Millisecond reactor with its corresponding TLE, showing the accuracy and ease of using COILSIM1D when dealing with simulations that explicitly link various aspects of the process altogether.

COILSIM1D comes with a user-friendly GUI, which makes it extremely easy to create and execute all types of simulations. The input and output files of the simulations are stored in Excel readable files, that can be easily imported into spreadsheets for further analysis and processing. This has the additional advantage of enabling easy interaction of COILSIM1D with user-created scripts for large batches of simulations, or to couple COILSIM1D to external software, e.g. to carry out whole-plant simulation and optimization.

The combination of all these new and already existing features enables users to perform accurate simulations of the whole furnace with limited number of inputs, reasonable computational effort and unprecedented accuracy, all with one click.

References

1. Van Geem, K. M.; Reyniers, M. F.; Marin, G. B., Challenges of modeling steam cracking of heavy feedstocks. *Oil & Gas Science and Technology-Revue D Ifp Energies Nouvelles* 2008, 63, (1), 79-94.
2. Hudebine, D.; Verstraete, J. J., Reconstruction of petroleum feedstocks by entropy maximization. Application to FCC gasolines. *Oil & Gas Science and Technology-Revue d'IFP Energies nouvelles* 2011, 66, (3), 437-460.
3. Van Geem, K. M.; Hudebine, D.; Reyniers, M. F.; Wahl, F.; Verstraete, J. J.; Marin, G. B., Molecular reconstruction of naphtha steam cracking feedstocks based on commercial indices. *Computers & Chemical Engineering* 2007, 31, (9), 1020-1034.
4. Pyl, S. P.; Van Geem, K. M.; Reyniers, M. F.; Marin, G. B., Molecular reconstruction of complex hydrocarbon mixtures: An application of principal component analysis. *AIChE journal* 2010, 56, (12), 3174-3188.
5. Dijkmans, T. Steam cracking: from feedstock analysis to plant optimization. Ghent University, 2014.
6. Lahaye, J.; Badie, P.; Ducret, J., Mechanism of carbon formation during steamcracking of hydrocarbons. *Carbon* 1977, 15, (2), 87-93.
7. Albright, L. F.; Marek, J. C., Mechanistic model for formation of coke in pyrolysis units producing ethylene. *Industrial & Engineering Chemistry Research* 1988, 27, (5), 755-759.
8. Kopinke, F. D.; Bach, G.; Zimmermann, G., New results about the mechanism of TLE fouling in steam crackers. *Journal of Analytical and Applied Pyrolysis* 1993, 27, (1), 45-55.
9. Muñoz Gandarillas, A. E.; Van Geem, K. M.; Reyniers, M. F.; Marin, G. B., Coking resistance of specialized coil materials during steam cracking of sulfur-free naphtha. *Industrial & Engineering Chemistry Research* 2014, 53, (35), 13644-13655.
10. Plehiers, P. M.; Reyniers, G. C.; Froment, G. F., Simulation of the run length of an ethane cracking Furnace. *Industrial & Engineering Chemistry Research* 1990, 29, (4), 636-641.
11. Reyniers, G. C.; Froment, G. F.; Kopinke, F.-D.; Zimmermann, G., Coke formation in the thermal cracking of hydrocarbons. 4. Modeling of coke formation in naphtha cracking. *Industrial & engineering chemistry research* 1994, 33, (11), 2584-2590.
12. Reyniers, M.-F. S.; Froment, G. F., Influence of metal surface and sulfur addition on coke deposition in the thermal cracking of hydrocarbons. *Industrial & engineering chemistry research* 1995, 34, (3), 773-785.
13. Muñoz Gandarillas, A. E.; Van Geem, K. M.; Reyniers, M. F.; Marin, G. B., Influence of the reactor material composition on coke formation during ethane steam cracking. *Industrial & Engineering Chemistry Research* 2014, 53, (15), 6358-6371.
14. Sabbe, M. K.; De Vleeschouwer, F.; Reyniers, M.-F.; Waroquier, M.; Marin, G. B., First principles based group additive values for the gas phase standard entropy and heat capacity of hydrocarbons and hydrocarbon radicals. *The Journal of Physical Chemistry A* 2008, 112, (47), 12235-12251.
15. Sabbe, M. K.; Reyniers, M. F.; Van Speybroeck, V.; Waroquier, M.; Marin, G. B., Carbon-Centered Radical Addition and β -Scission Reactions: Modeling of Activation Energies and Pre-exponential Factors. *ChemPhysChem* 2008, 9, (1), 124-140.

16. Sabbe, M. K.; Reyniers, M. F.; Waroquier, M.; Marin, G. B., Hydrogen Radical Additions to Unsaturated Hydrocarbons and the Reverse β -Scission Reactions: Modeling of Activation Energies and Pre-Exponential Factors. *ChemPhysChem* 2010, 11, (1), 195-210.
17. Sabbe, M. K.; Vandeputte, A. G.; Reyniers, M.-F.; Waroquier, M.; Marin, G. B., Modeling the influence of resonance stabilization on the kinetics of hydrogen abstractions. *Physical Chemistry Chemical Physics* 2010, 12, (6), 1278-1298.
18. Saeys, M.; Reyniers, M. F.; Marin, G. B.; Van Speybroeck, V.; Waroquier, M., Ab initio group contribution method for activation energies for radical additions. *AIChE journal* 2004, 50, (2), 426-444.
19. Saeys, M.; Reyniers, M. F.; Van Speybroeck, V.; Waroquier, M.; Marin, G. B., Ab initio group contribution method for activation energies of hydrogen abstraction reactions. *ChemPhysChem* 2006, 7, (1), 188-199.
20. Van Geem, K. M.; Reyniers, M.-F.; Marin, G. B. In *Taking optimal advantage of feedstock flexibility with COILSIM1D*, AIChE Spring Meeting: Ethylene producers conference, New Orleans, LA, USA, 2008; New Orleans, LA, USA, 2008.
21. Zimmermann, H.; Walzl, R., Ethylene. *Ullmann's Encyclopedia of Industrial Chemistry* 2009.
22. Heynderickx, G. J. Modelling en Simulatie van Huidige en Nieuwe Technologieën voor de Thermische Kruiging van Koolwaterstoffen. University Ghent, Ghent, 1993.