ONE STEP KINETIC MODEL
OF COAL PYROLYSIS FOR CFD APPLICATIONS

T. Maffei, E. Ranzi, A. Frassoldati, T. Faravelli
tiziano.faravelli@polimi.it
Dipartimento di Chimica, Materiali e Ingegneria Chimica, Politecnico di Milano, Italy

Abstract
This work’s aim is the development of a simplified kinetic model for coal devolatilization, suitable for CFD applications. The detailed model of coal devolatilization, already developed and tested against a very large set of experiments and conditions, is too large to be easily implemented and used inside a CFD code.
An automatic procedure is developed to estimate the kinetic parameters and stoichiometric coefficients of a One Step model. An optimization technique manages to minimize an objective function which measures the distance between the simple one step kinetic mechanism and the results of a detailed model for coal devolatilization. One of the important features of this approach is that, thanks to the optimizer, it is possible to easily calculate specific rate parameters for each type of coal. Moreover the one step model, despite its simplicity, is able to characterize not only the coal consumption but also the relative yields of gaseous species (H$_2$O, CO$_2$, H$_2$, HCN, H$_2$S, H$_2$, C$_2$H$_4$), tar species and solids species. The coal database includes 13 coals of different elemental composition, from lignite to anthracite. The agreement of the one step model with the detailed model of coal volatilization is satisfactory for both evolution rates and cumulative values. Moreover it is important to note that the proposed model, being based on the detailed model, is predictive and only needs the coal elemental composition (coal rank) as an input. A correlation for the distribution of the nitrogen and sulfur compounds into solid, tar and gas phases is also proposed.

Introduction
The investigation of coal combustion equipments is complex because it involves both kinetic aspects (coal devolatilization, char and gas oxidation) and physical aspects. Due to a combination of increased computer power and advanced numerical techniques, the use if Computational Fluidynamics (CFD) simulations is increasing and offers the possibility to study the interaction of physical and chemical processes involved in coal combustion. The resulting simulations can help to optimize the system design and operation and minimize the formation of pollutants. Unfortunately, the direct coupling of detailed kinetic mechanisms and CFD simulations makes the computational cost prohibitive in the case of real combustors, characterized by large computational grids. For this reason, it is important to develop simple but reliable kinetic mechanism for coal
devolatilization to be used in CFD modeling. Devolatilization is the first step in coal combustion, thus an accurate kinetic modeling is relevant for the optimal design of these processes. In this work we developed a One Step mechanism for coal devolatilization able not only to describe the conversion of coal but also the relative yields of gaseous, tar and solids species. Moreover, the release of nitrogen and sulphur compounds during coal pyrolysis is described by the model.

**Detailed Model of Coal Pyrolysis**

Detailed models for coal devolatilization were already developed and tested against a very large set of experiments and conditions. More specifically, three different detailed kinetic models are involved in coal devolatilization:

1. Kinetic model for the release of Hydrocarbon species
2. Kinetic model for the release of Sulfur compounds
3. Kinetic model for the release of Nitrogen compounds

The details of the first two kinetic models are described in detail in [1] and [2], while the last one is briefly presented in this paper. An automatic procedure is used to estimate the kinetic parameters and stoichiometric coefficients of a simple One Step model on the basis of the detailed mechanism.

**Nitrogen Kinetic Model**

In coals, nitrogen is present in different forms (quaternary, pyridinic and pyrolytic compounds [3,4]), but these species do not show an evident correlation with the elemental composition or others physical properties of coals. Experimental information [5, 6] showed that similar behaviors for nitrogen volatile compounds and total volatile matter released from coals in pyrolytic conditions. On the basis of this information and to maintain a consistency in the model, we adopted for the nitrogen matrix the same criterion already used to characterize the effect of the solid phase composition on the release of hydrocarbon species. The nitrogen solid references compounds are COAL1-N, COAL2-N, COAL3-N, CHAR-N, tightly tied to reference compounds COAL1, COAL2, COAL3, CHAR (see [1] for details). The mechanism includes low temperature (with activation energy of 33-40 kcal/mol) and high temperature reactions (61-75 kcal/mol), and also cross-linking and annealing reactions. At low heating rates conditions, the products are not directly released to the gas phase but they are entrapped in the metaplastic phase (NH₃*, HCN*, NTAR*). These species are finally released to the gas phase only at higher temperatures (NH₃, HCN, NTAR). At high temperatures (or high heating rates), the nitrogen species are directly released to the gas phase. This multi–step kinetic mechanism contains 11 species involved in 17 reactions and is reported in table 1. Figure 1 shows the comparison between experimental data and model prediction, at low (panel a) and high (panel b) heating rate conditions.
Table 1. Multi-steps kinetic model of nitrogen release.

<table>
<thead>
<tr>
<th>Step</th>
<th>Reaction</th>
<th>Rate Constant</th>
<th>Arrhenius Parameter</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>COAL-N₁ → 0.1 NH₃⁺ + 0.05 HCN⁺ + 0.85 NCHAR</td>
<td>9.0×10⁷</td>
<td>40000</td>
</tr>
<tr>
<td>2</td>
<td>COAL-N₁ → N₅AR⁺</td>
<td>1.0×10⁸</td>
<td>40000</td>
</tr>
<tr>
<td>3</td>
<td>COAL-N₁ → 0.05 NH₃ + 0.3 HCN + 0.65 NCHAR</td>
<td>1.6×10¹⁵</td>
<td>75000</td>
</tr>
<tr>
<td>4</td>
<td>COAL-N₁ → N₅AR</td>
<td>1.0×10¹⁴</td>
<td>75000</td>
</tr>
<tr>
<td>5</td>
<td>COAL-N₂ → 0.15 NH₃⁺ + 0.03 HCN⁺ + 0.82 NCHAR</td>
<td>7.6×10¹⁰</td>
<td>36000</td>
</tr>
<tr>
<td>6</td>
<td>COAL-N₂ → N₅AR⁺</td>
<td>5.0×10¹⁰</td>
<td>36000</td>
</tr>
<tr>
<td>7</td>
<td>COAL-N₂ → 0.15 NH₃ + 0.3 HCN + 0.55 NCHAR</td>
<td>3.0×10¹⁷</td>
<td>63000</td>
</tr>
<tr>
<td>8</td>
<td>COAL-N₂ → N₅AR</td>
<td>4.0×10¹⁷</td>
<td>63000</td>
</tr>
<tr>
<td>9</td>
<td>COAL-N₃ → 0.15 NH₃⁺ + 0.15 HCN⁺ + 0.7 NCHAR</td>
<td>4.0×10¹⁰</td>
<td>33000</td>
</tr>
<tr>
<td>10</td>
<td>COAL-N₃ → N₅AR⁺</td>
<td>1.6×10⁹</td>
<td>33000</td>
</tr>
<tr>
<td>11</td>
<td>COAL-N₃ → 0.15 NH₃ + 0.1 HCN + 0.75 NCHAR</td>
<td>5.0×10¹⁸</td>
<td>61000</td>
</tr>
<tr>
<td>12</td>
<td>COAL-N₃ → N₅AR</td>
<td>2.0×10¹⁸</td>
<td>61000</td>
</tr>
<tr>
<td>13</td>
<td>NCHAR + N₅AR → 0.05 NH₃ + 0.1 HCN + 1.85 NCHAR</td>
<td>2.1×10⁶</td>
<td>32500</td>
</tr>
<tr>
<td>14</td>
<td>N₅AR⁺ → N₅AR</td>
<td>3.0×10⁸</td>
<td>32500</td>
</tr>
<tr>
<td>15</td>
<td>NH₃⁺ → NH₃</td>
<td>1.0×10³</td>
<td>23000</td>
</tr>
<tr>
<td>16</td>
<td>HCN⁺ → HCN</td>
<td>4.0×10²</td>
<td>23000</td>
</tr>
<tr>
<td>17</td>
<td>NCHAR → CHAR + HCN</td>
<td>2×10⁹</td>
<td>80000</td>
</tr>
</tbody>
</table>

(*) $k = A \exp(-E_{ATT}/RT)$ (Units are kcal, kmol, m, K, s)

Figure 1. (a) Release of N as NH₃ and HCN as a function of coal rank (%w C, daf); (b) Release of total volatile nitrogen. Symbols: experimental data (a) [7] (b) [8,9]; line with symbols: model predictions ($w_{N,species}/w_{N_{0_{coal}}}$)

The complete model for coal devolatilization contains the hydrocarbon scheme combined with the nitrogen and sulphur kinetic model, and is constituted of ~60 species and ~70 reactions. As already discussed this model is too complex for a direct use inside CFD codes, in fact the cost of a simulation would be prohibitive for real combustors characterized by large computational grids. Therefore, simplified models are required and the development of a one step kinetic scheme is presented in this paper.
One Step Model
An automatic procedure estimates the kinetic parameters and stoichiometric coefficients of a 1-Step model:

\[
COAL \rightarrow Char + TAR + CO + CO_2 + H_2O + H_2 + C_2H_4 + H_2S + HCN \quad k = A \times e^{\frac{E}{RT}}
\]

Char is characterized just in terms of C, N and S atoms, while tar contains C, H, O, N and S hetero-atoms.

An optimization technique manages to minimize an objective function which measures the distance between the simple one step kinetic mechanism and the results of a detailed model for coal volatilization:

\[
S(b) = \sum_{i=1}^{n_e} \sum_{k=1}^{n_y} \left[ (y_{i,k} - g_k(x_i, b)) \right]^2
\]

\(n_e\) is the number of experimental point, \(n_y\) is the number of dependent variable \(y_i\), while \(x_i\) are the independent variable. \(b\) is a vector of parameters and \(g_k\) are the kinetic equations.

The BzzNonLinearRegression class, of BzzMath 6.0 (Buzzi-Ferraris, http://homes.chem.polimi.it/gbuzzi/) has been used to find the minimum of the objective function.

The complete detailed model is used as a generator of dummy ‘experimental data’, in opportune simulation condition, typically those that occur in a oxy-coal furnace (high heating rate of \(\sim 10^4\) K/s and temperatures larger than 1400 K).

As mentioned, the coal database for ‘experimental data’ creation includes 13 coals of different elemental composition, from lignite to anthracite. Figure 2 shows the results of the non-linear regression process in terms of the logarithm of pre-exponential factor and activation energy as a function of coal carbon content.

![Figure 2](image)

**Figure 2.** Frequency factor (a) and activation energy (b) as a function carbon [%] in coal. Units are s, kcal, kmol.

It is possible to observe from figure 2 that there is a linear correlation between logarithm of pre-exponential factor and carbon content, and an exponential correlation between the activation energy and the same independent variable. These correlation are:

\[
\log_{10} A = 22.12 - 0.067 \times C_{\%} \quad E = 5.67 \times 10^{-3} e^{6.35} + 55653
\]
Table 2. Decomposition products for each reference coal (kmol j-th species per kmol of reference coal).

<table>
<thead>
<tr>
<th></th>
<th>CHAR C</th>
<th>H&lt;sub&gt;2&lt;/sub&gt;</th>
<th>CH&lt;sub&gt;4&lt;/sub&gt;</th>
<th>C&lt;sub&gt;2&lt;/sub&gt;H&lt;sub&gt;5&lt;/sub&gt;</th>
<th>BTEX</th>
<th>CO</th>
<th>H&lt;sub&gt;2&lt;/sub&gt;O</th>
<th>CO&lt;sub&gt;2&lt;/sub&gt;</th>
<th>TAR&lt;sub&gt;1&lt;/sub&gt;</th>
<th>TAR&lt;sub&gt;2&lt;/sub&gt;</th>
<th>TAR&lt;sub&gt;3&lt;/sub&gt;</th>
</tr>
</thead>
<tbody>
<tr>
<td>COAL&lt;sub&gt;1&lt;/sub&gt;</td>
<td>5.13</td>
<td>1.50</td>
<td>0.38</td>
<td>0.50</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.50</td>
<td>0.00</td>
<td>0.00</td>
</tr>
<tr>
<td>COAL&lt;sub&gt;2&lt;/sub&gt;</td>
<td>9.41</td>
<td>2.69</td>
<td>0.32</td>
<td>0.10</td>
<td>0.15</td>
<td>0.82</td>
<td>0.09</td>
<td>0.00</td>
<td>0.10</td>
<td>0.09</td>
<td>0.00</td>
</tr>
<tr>
<td>COAL&lt;sub&gt;3&lt;/sub&gt;</td>
<td>3.64</td>
<td>1.35</td>
<td>0.26</td>
<td>0.59</td>
<td>0.11</td>
<td>1.91</td>
<td>0.64</td>
<td>0.09</td>
<td>0.00</td>
<td>0.29</td>
<td></td>
</tr>
<tr>
<td>CHAR&lt;sub&gt;c&lt;/sub&gt;</td>
<td>1.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
<td>0.00</td>
</tr>
</tbody>
</table>

In oxy-coal combustion conditions, the high temperature mechanism is the dominant one. Table 2 shows the predicted high temperature decomposition products for each reference coal. The stoichiometric coefficients for the decomposition products of a coal of known elemental composition are then calculated by simply weighing the molar contribution of each reference coal (COAL<sub>i</sub>). In fact, as already discussed in detail by Sommariva et al. [1], each coal can be represented by a proper combination of the four reference species.

\[
\alpha_j = (100 - N_{\%} - S_{\%}) \times \sum_{i=1}^{N_{\text{COAL}}} \omega_{\text{COAL}_i,j} \times \alpha_{\text{COAL}_i,j} \\
\alpha_{\text{TAR},i} = \frac{(100 - N_{\%} - S_{\%})}{PM_{\text{TAR}}} \times \sum_{j=1}^{N_{\text{TAR}}} PM_j \times \frac{4 \omega_{\text{COAL}_i,j} \times \alpha_{\text{COAL}_i,j}}{PM_{\text{TAR}}} \\
\]

Where \( \alpha_j \) is the stoichiometric coefficient for j-th species in the One Step model, N\% and S\% are the mass \% of nitrogen and sulphur in coal, \( \omega_{\text{COAL}_i} \) is the mass fraction of i-th reference coals, \( \alpha_{\text{COAL}_i,j} \) is the stoichiometric coefficient of j-th species for i-th reference coal in table 2, PM<sub>COAL</sub> is the molecular weight of i-th reference coals (COAL<sub>1</sub>=C<sub>12</sub>H<sub>11</sub>, COAL<sub>2</sub>=C<sub>14</sub>H<sub>10</sub>O, COAL<sub>3</sub>=C<sub>12</sub>H<sub>12</sub>O<sub>5</sub>, CHAR<sub>c</sub>=C), PM<sub>i</sub> is the molecular weight of j-th tar species (TAR<sub>1</sub>= C<sub>12</sub>H<sub>11</sub>, TAR<sub>2</sub>= C<sub>14</sub>H<sub>10</sub>O, TAR<sub>3</sub>= C<sub>11</sub>H<sub>10</sub>O<sub>2</sub>) and PM<sub>TAR</sub> is the molecular weight of TAR specie. The elemental composition of TAR<sub>CHO</sub> is calculated as follows:

\[
C_{\text{TAR}} = \sum_{i=1}^{N_{\text{TAR}}} x_{\text{TAR}_i} \times C_{\text{TAR}_i} \\
H_{\text{TAR}} = \sum_{i=1}^{N_{\text{TAR}}} x_{\text{TAR}_i} \times H_{\text{TAR}_i} \\
O_{\text{TAR}} = \sum_{i=1}^{N_{\text{TAR}}} x_{\text{TAR}_i} \times O_{\text{TAR}_i} \\
x_{\text{TAR}} = \frac{\sum_{i=1}^{N_{\text{COAL}}} \omega_{\text{COAL}_i} \times \alpha_{\text{TAR},i} \times \alpha_{\text{COAL}_i,j}}{\sum_{i=1}^{N_{\text{TAR}}} \sum_{j=1}^{N_{\text{TAR}}} \omega_{\text{COAL}_i,j} \times \alpha_{\text{COAL}_i,j}}
\]

where x<sub>TAR</sub><sub>i</sub> are the molar fraction of i-th tar components in tar mixture, C<sub>TAR</sub><sub>i</sub>, H<sub>TAR</sub><sub>i</sub>, O<sub>TAR</sub><sub>i</sub>, are respectively carbon, hydrogen and oxygen content in the i-th TAR<sub>i</sub>, and \( \alpha_{\text{TAR},i} \) are the stoichiometric coefficient of TAR<sub>i</sub> compound in table 2.

Table 3. Correlation of repartition for nitrogen and sulphur compounds into solid, tar and gas phase.

<table>
<thead>
<tr>
<th>Nitrogen Repartition*</th>
<th>Sulphur Repartition*</th>
</tr>
</thead>
<tbody>
<tr>
<td>( N_{\text{TAR}} ) = -6.56 + 0.177×C% - 1.13×10^{-3}×C^2 %</td>
<td>( S_{\text{TAR}} ) = -2.48 - 5.49×10^{-2}×C% + 3.45×10^{-4}×C^2 %</td>
</tr>
<tr>
<td>( N_{\text{CHAR}} ) = 7.3 - 0.175×C% + 1.12×10^{-3}×C^2 %</td>
<td>( S_{\text{CHAR}} ) = -1.20 + 3.48×10^{-2}×C% - 2.182×10^{-4}×C^2 %</td>
</tr>
<tr>
<td>( N_{\text{GAS}} ) = 1 - ( N_{\text{TAR}} ) - ( N_{\text{CHAR}} )</td>
<td>( S_{\text{GAS}} ) = 1 - ( S_{\text{TAR}} ) - ( S_{\text{GAS}} )</td>
</tr>
</tbody>
</table>

*Kg N o S in j phase respect initial nitrogen or sulphur content in coal. j = CHAR, TAR, GAS
Closure of H and C atomic balance is obtained by introducing an opportune mixture of C_{x}H_{y}, whose composition depends not only on the difference between initial content of carbon and hydrogen in the coal and carbon and hydrogen into TAR, CO, CO_{2}, H_{2}O, but also of the amount of carbon and hydrogen associate with nitrogen and sulfur released in the gas phase. The oxygen balance is always satisfied because the total amount oxygen has been already counted for in inorganic oxygen specie (CO, CO_{2}, H_{2}O) and in TAR compound.

Figure 3 shows sulphur and nitrogen repartition between solid, tar and gas phases in function of carbon content in the parent coal. These distributions are obtained from the detailed kinetic model in the same simulation conditions already used for the One Step model. The associated correlations are reported in table 3.

**Solid Phase**

The solid residue reference species \( \text{CHAR}_{\text{Coal}} \) contains C, N, S. The stoichiometric coefficient in the One Step model is \( \alpha_{\text{CHAR},\text{Coal}} \), obtained from equation 3, while the brute formula is \( \text{C}_{1}x_{\text{N}}y_{\text{S}} \) where

\[
x = N_{\text{CHAR}} \times \omega_{\text{N}}^{\text{COAL}} \times \frac{\text{PM}_{\text{COAL}}}{\text{PM}_{N}} \times \frac{1}{\alpha_{\text{CHAR}}} \quad y = S_{\text{CHAR}} \times \omega_{\text{S}}^{\text{COAL}} \times \frac{\text{PM}_{\text{COAL}}}{\text{PM}_{S}} \times \frac{1}{\alpha_{\text{CHAR}}} \tag{6}
\]

where \( N_{\text{CHAR}} \) and \( S_{\text{CHAR}} \) are the repartition of nitrogen and sulphur in the solid phase (see table 2). The elemental composition of each coal is calculated from the normalized daf elemental composition. PM_{N} and PM_{S} are the respectively molecular weight of nitrogen and sulphur.

**Tar Phase**

The TAR reference species \( \text{TAR}_{\text{Coal}} \) contains C, H, O, N, S. The stoichiometric coefficient of this species in the one step model is \( \alpha_{\text{TAR},\text{Coal}} \) and is obtained from equation 4. The brute formula is \( \text{C}_{x}\text{H}_{y}\text{O}_{z}\text{N}_{k}\text{S}_{j} \) where \( x, y, z \) are defined in equation 5, while and \( k \) and \( j \) are:
\[ k = N_{\text{TAR}} \times \frac{\omega^N_{\text{COAL}}}{\alpha_{\text{TAR}}} \times \frac{PM_{\text{COAL}}}{PM_N} \times \frac{1}{\alpha_{\text{TAR}}} \]
\[ j = S_{\text{TAR}} \times \frac{\omega^S_{\text{COAL}}}{\alpha_{\text{TAR}}} \times \frac{PM_{\text{COAL}}}{PM_S} \times \frac{1}{\alpha_{\text{TAR}}} \]  

where \( N_{\text{TAR}} \) and \( S_{\text{TAR}} \) are the repartition of nitrogen and sulphur in the tar phase, as reported in table 2.

**Gas Phase**

It is necessary to add the contribution of nitrogen and sulphur gas compounds to the release of gas species. HCN and \( \text{H}_2\text{S} \) can be used as representatives of \( \text{NGAS} \) and \( \text{SGAS} \) (they are the major products in the high temperature condition [5,10]). The closure of the atomic balances for C and H requires to know the amount of HCN and \( \text{H}_2\text{S} \) released (i.e. their stoichiometric coefficients). In this way it is possible to evaluate the stoichiometric coefficient of the \( \text{C}_x\text{H}_y \) mixture by imposing to satisfy the atomic balance. The \( \text{C}_x\text{H}_y \) is a mixture of \( \text{C}_2\text{H}_4 \) and \( \text{H}_2 \):

\[ \alpha_j = (100 - N_N - S_S) \times \sum \frac{\omega^N_{\text{COAL}}}{\alpha_{\text{COAL}}} \times \alpha_{\text{COAL}} \]
\[ j = \text{CO}, \text{CO}_2, \text{H}_2\text{O} \]  

\[ \alpha_{\text{H}_2} = \frac{S_{\text{GAS}} \times PM_{\text{COAL}}}{PM_S} \]
\[ \alpha_{\text{HCN}} = \frac{N_{\text{GAS}} \times PM_{\text{COAL}}}{PM_N} \]
\[ \Delta C = \omega^{C}_{\text{GAS}} - PM_C \times \sum \frac{\omega^N_{\text{COAL}}}{\alpha_{\text{COAL}}} \times \alpha_{\text{COAL}} \]
\[ \Delta H = \omega^{H}_{\text{GAS}} - PM_H \times \sum \frac{\omega^N_{\text{COAL}}}{\alpha_{\text{COAL}}} \times \alpha_{\text{COAL}} \]
\[ \alpha_{\text{C}_2\text{H}_4} = \frac{PM_{\text{COAL}}}{2} \times \frac{\Delta C}{PM_C} \times \frac{1}{2} \alpha_{\text{HCN}} \]
\[ \alpha_{\text{H}_2} = \frac{PM_{\text{COAL}}}{2PM_H} \Delta H - 2 \times \alpha_{\text{C}_2\text{H}_4} \times \frac{1}{2} \alpha_{\text{NGAS}} - \alpha_{\text{H}_2} \]  

where \( \text{NGAS} \) and \( \text{SGAS} \) are the repartition of nitrogen and sulphur in the gas phase (table 2).

**Figure 4.** Comparison between detailed model and One Step model for three different coal at 1500 and 1800 K in term of nitrogen and sulphur repartition (heating rate of \( 10^4 \text{K/s} \)).

Figure 4 and 5 show the comparison between the original detailed model and the One Step model developed in this work. The agreement of the one step model with the detailed model is satisfactory for both evolution rates and cumulative values. The main difference is the more direct release of species in the case of the One
Step model (in the detailed model several species are not directly released but are entrapped in metaplastic phase at low temperatures). A second difference lies in the low temperature mechanism accounted for in the detailed model. It is important to note that the proposed model, being based on the detailed model, is predictive and only needs the coal elemental composition (coal rank) as an input. A correlation for the distribution of the nitrogen and sulfur compounds into solid, tar and gas phases is also proposed.

As an example, the One Step kinetic model for devolatilization of the Liddel coal is:

\[
Liddel \rightarrow 4.146 \text{CHAR}_{\text{Coal}} + 0.144 \text{TAR}_{\text{Coal}} + 0.356 \text{CO} + 0.022 \text{CO}_2 + 0.074 \text{H}_2\text{O} + 1.21 \text{H}_2 + 0.317 \text{C}_2\text{H}_4 + 0.017 \text{HCN} + 0.003 \text{H}_2\text{S}
\]

\[
k = 3.6 \times 10^{16} \times e^{-\frac{58600}{RT}}
\]

![Comparison between detailed model (red lines) and One Step model (blue lines) for three different coals at 1500 and 1800 K in term of hydrocarbon species (heating rate of 10^4 K/s).](image)

**Figure 5.** Comparison between detailed model (red lines) and One Step model (blue lines) for three different coals at 1500 and 1800 K in term of hydrocarbon species (heating rate of 10^4 K/s).

**Conclusion**

In this work a simplified model for coal devolatilization has been developed. This mechanism is suitable for CFD simulations. It was developed using a detailed model [1,2] and a non linear regression technique to estimate the optimal kinetic parameters and stoichiometric coefficients. The agreement with detailed model is satisfactory for both evolution rates and cumulative values. This One Step model, despite its simplicity, retains the predictive capabilities of the original detailed
model for the formation of solid, tar and gaseous species, including sulfur and nitrogen compounds..

**Acknowledgments**
This work is funded in the frame of the ‘Accordo di Programma Ministero dello Sviluppo Economico –ENEA’.

**References**
[6] Perry S.T., Ph.D thesis, Brigham Young University, Utah, USA.