Emission inventory supported by $R$

dependency between calorific value and carbon content for lignite.

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Introduction I

The beginning – Convention on the Climate Change (UNFCCC)

- COP 1 – Berlin Mandate (1995) 🇩🇪
  Annex I countries (including EiT) – 41 countries,
  Non-Annex I countries – developing countries;
- COP 3 – Kyoto Protocol (1997) 🇯🇵
  ratified by Russian Federation (2004),
  entered into force (2005) (...);
- COP 14 – Poznań (2008) 🇵🇱
Activities connected with the Convention on the Climate change ”have begun” in 1992 in Rio de Janeiro;

The Berlin Mandate (1995) distinguished Annex I countries (responsible for historical emissions of GHGs);

The emission inventory is one of obligations under UNFCCC;

Under Kyoto Protocol, Annex I countries are obliged to reduce emissions of GHGs (CO₂ i.a.).
Why analysis of lignite? I

Structure of fuels used in utility plants in Poland¹ years: 1988–2011

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¹Electricity and heat production – gross consumption of fuels.
Why analysis of lignite? II

According to the available sources of information:

- **Share** of lignite combusted in public utility plants\(^2\) in Poland is estimated as **32–35%** (years: 2000–2011) \([3, 4]\);
- Development of **exploiting** of sources of lignite in Poland is forecasted till **2038** \([8]\) or even almost **2100** \([7]\);
- Sometimes **application** of **CCS** technology **could be problematic** (Bełchatów, Poland) \(\text{source}\);
- Current **Polish methodology** of estimation of CO\(_2\) emission from combustion of lignite **should be updated** due to availability of new pieces of information.

\(^2\) public energy and heat production sector.
Current methodology

How to? I

Everything that can be thought at all can be thought clearly.

Everything that can be said can be said clearly.

L. Wittgenstein

Emission estimation:

\[ E_{\text{combustion}}^{\text{lignite}} = A \cdot EF_{\text{CO}_2} \]

\( A \) – activity of emission source (Mg of lignite mined, amount of electricity or heat produced);

\( EF \) – \( \text{CO}_2 \) emission factor (average mass of \( \text{CO}_2 \) produced from particular mass of combusted lignite or amount of electricity or heat produced).
What is (really) the CO₂ emission factor in case of carbon-based fuel?

- Let’s check it:
  - \( \text{C} + \text{O}_2 \rightarrow \text{CO}_2 \) – equation of CO₂ production during combustion
  - **Carbon content in fuel generates production of CO₂**
  - **12 kg of pure carbon creates (with oxygen) 44 kg of CO₂**

Fott [5] found linear dependency between calorific value and carbon content in case of hard coal and lignite.
Current methodology

Fott’s approach

According to Fott’s findings [5]:

- There is found strong linear correlation between NCV\(^3\) and carbon content in hard coal or lignite;
- The accuracy of CEF\(^4\) determination is better for hard (bituminous) coal than for brown coal (lignite);

The last finding suggests bigger variability of parameters of the lignite.

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\(^3\) Net Calorific Value, lower heating value, e.g. [MJ/kg].

\(^4\) Carbon Emission Factor [t C/TJ].
Current methodology

Fott’s approach II

Formulas of dependency found by Fott [5]:

- wet coal and lignite: \( c_t^\prime = 2.400 \cdot Q_i^\prime + 4.1232 \);
- dry and ash removed coal and lignite: \( c_t^\prime = 2.333 \cdot Q_i^\prime + 5.511 \);
- selected country specific values: \( c_t^\prime = 2.334 \cdot Q_i^\prime + 5.5786 \);
- set ”A+B”: \( c_t^\prime = 2.344 \cdot Q_i^\prime + 5.056 \);

\( c_t^\prime \) – total carbon content [%]
\( Q_i^\prime \) – Net Calorific Value (NCV) [MJ/kg]
Current methodology

Current Polish methodology

**Current Polish methodology is based on the Fott’s approach**, there are found two types of linear dependency between carbon content and NCV [10]^5:

- for hard coal: \( c_t^r = 2.4898 \cdot Q_i^r + 3.3132; \)
- for lignite: \( c_t^r = 1.9272 \cdot Q_i^r + 9.3856. \)

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^5 Original elaboration by: Olendrzyński et al., is not published
According to findings done by Stefanović et al. [11, 12], there are created similar linear functions describing dependence between calorific values and carbon content in lignite\(^6\):

- Šoštanj power plant: \( c_t^r = 2.2477 \cdot Q_i^r + 5.8216 \);
- Velenje: \( c_t^r = 2.3878 \cdot Q_i^r + 4.6548 \);
- Kolubara: \( c_t^r = 1.9272 \cdot Q_i^r + 4.2637 \).

\(^6\)Apart from that, we’ve done our little analysis – coming soon [14].
Assumptions I

Basing on modified Dulong formula [9]:

\[ CV_D = 340.80c + 1427.70(h - \frac{o}{8}) + 92.20s - 25.50(w + 9h) \]  \hspace{1cm} (1)

where:
\( c, h, o, s, w, p \) – mass fractions of: carbon, hydrogen, oxygen, sulphur, water (moisture) and ash

Formula for lignite "as derived":

\[ c + (p + s + w) + n + h + o = 100\% \]  \hspace{1cm} (2)
Assumptions II

Basing on [1, 13]: $p \approx 9\%, s \approx 1\%, w \approx 56\%$.

$p + s + w = 66\%$ (as derived)

and with dry and ash removed

$(h^{\text{daf}} \approx 6\%, n^{\text{daf}} \approx 1\%, o^{\text{daf}} \approx 20\%)$:

\[ c + n + h + o = 34\% \] (3)

\[
\begin{array}{cccc}
73\% & 1\% & 6\% & 20\% \\
25\% & 0.34\% & 2\% & 7\%
\end{array}
\]
Assumptions III

Findings for Bełchatów mining field [2]:

\[ w \% \sim N(\mu_w, \sigma_w) = N(56.30, 1.53); \]
\[ s'_t \% \sim N(\mu_{s'_t}, \sigma_{s'_t}) = N(0.20, 0.02) \rightarrow \text{sulphur content total lignite as derived (wet)}; \]
\[ CV \ [kJ/kg] \sim N(\mu_{CV}, \sigma_{CV}) = N(8010.73, 415.75) \ [kJ/kg]. \]

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7 Analysis carried out for 63 samples from Bełchatów mining field – found normal distributions.
8 Converted from [kcal/kg].
As in equations (1) & (2):

$$340.80c = CV_D - 1427.70\left(h - \frac{o}{8}\right) - 92.20s + 25.50(w + 9h)$$  \hspace{2cm} (4)$$

$$c = \frac{CV_D}{340.80} - 0.2705s + 0.0748w - 3.516h + 0.5237o$$  \hspace{2cm} (5)$$

Assuming the normal distribution of variables: $h$ and $o$, the variable $c$ has the normal distribution.

As in equation (3) estimated $h \approx 2\%$ and $o \approx 7\%$, then:

$$c = \frac{CV}{340.80} - 0.2705s_t^r + 0.0748w - 0.0337, \quad CV_D \rightarrow CV, \quad s \rightarrow s_t^r$$  \hspace{2cm} (6)$$
Still linear dependency

cv <- rnorm(10000,8010.73,415.75) #;cv
s <- rnorm(10000,0.2,0.02) #;s
w <- rnorm(10000,0.563,0.0153) #;w
c <- cv/340.8-0.2705*s+0.0748*w-0.0337 #;c
> lm(c ~ cv)
Call:
  lm(formula = c ~ cv)
Coefficients:
  (Intercept)   cv
-0.043416   0.002934 → for CV[kJ/kg]

for CV[MJ/kg]:  
  \[ c'_r = 2.934 \cdot Q'_i - 0.043416; \]
Currently used formula:  
  \[ c'_r = 1.9272 \cdot Q'_i + 9.3856 \]
Monte Carlo simulation

For 1000 samples. `c.norm <- (c-mean(c))/sd(c)` #By analogy for 1000 samples
Advantages

😊 Model is simple and can be easily developed by adding new information about lignite (e.g. parameters, resources, time of mining from particular field or any other);

😊 We can generate some parameters without carrying out specific analysis (e.g. chemical);

😊 We can quickly calculate uncertainties;

😊 Good for engineering purposes.
Disadvantages

- The assumptions say that the variables: $c$, $s$, $w$, $h$ and $o$ are uncorrelated – we can introduce particular correlations between variables, but it makes model more and more complicated;

- Model doesn’t take into consideration differences between export and import of lignite.
Thank you for your attention 😊

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References III
