Approximation Models of Phenomena at Gas Blowing into Ladle

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Abstract: *The paper describes the physical and cybernetic approach to the task of looking for an appropriate approximation-regression model of the measured standardised concentration of the tracer at a scale physical model of the casting ladle when basting the steel by inert gas. The physical approach allows assembling an adequate mathematical model of the processes in the shape of a so-called white box, where the structure of the model are known. The cybernetic approach only draws on the measured inputs and outputs (so-called black box) as well as any additional conditions (so-called grey box) and the structure of the model is chosen according to them. These models are referred to as empirical models. The paper presents and compares four models – a physically adequate one and three empirical ones.*

Keywords: *physical model, physical approach, cybernetic approach, physically adequate model, empirical models*

1 Introduction

For the measured time path of tracer concentrations in the physical model of the ladle (L) at blowing of steel by inert gas (argon) it was appropriate to construct physical-mathematical (physically adequate) and empirical models. Four developed models were verified with use of parametric simulation identification and non-linear regression analysis and their outputs were compared.

Results of these analyses can be used for setting of suitable mode of operation for blowing, as well as for teaching at technical universities.

2 Description of situation

Schematic illustration at blowing of steel (water) by inert gas (argon) in the model of the ladle (hereinafter *mL*, which was created on a geometric scale 1:10) is shown in *Figure 1*:
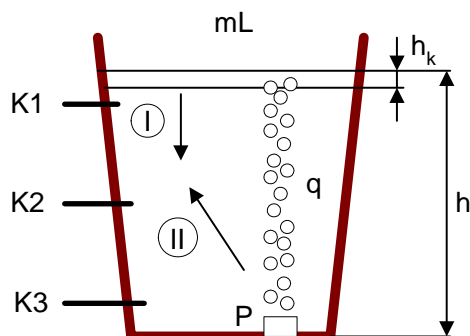

Figure 1 – Blowing of argon into the ladle model

Into the vessel of the *mL* three conductive sensors are inserted - *K1*, *K2* and *K3*. Bubbles

of inert gas (argon) with constant volume flow q are flowing from the blowing element P (blowing block) situated eccentrically at the bottom of the mL. They „erode" the layer of coloured water enriched in concentration with the height (thickness) h_k and there occurs gradual progressive stirring up of enriched and clear liquid (steel, water). Two (pressure) forces I and II work basically against each other on molecules of water in proximity of the sensors.

3 Measured data

Analysis and synthesis of physical-mathematical model was made on the basis of the experiment realised on 12th May 2006, where the development of the measured concentrations $c_i(t)$, i ∈ {1,2,3}, (with sampling period $\Delta t \approx 0.5$ s), in the sensors $K1$, $K2$ and $K3$ had the following shape – see *Figure 2*:

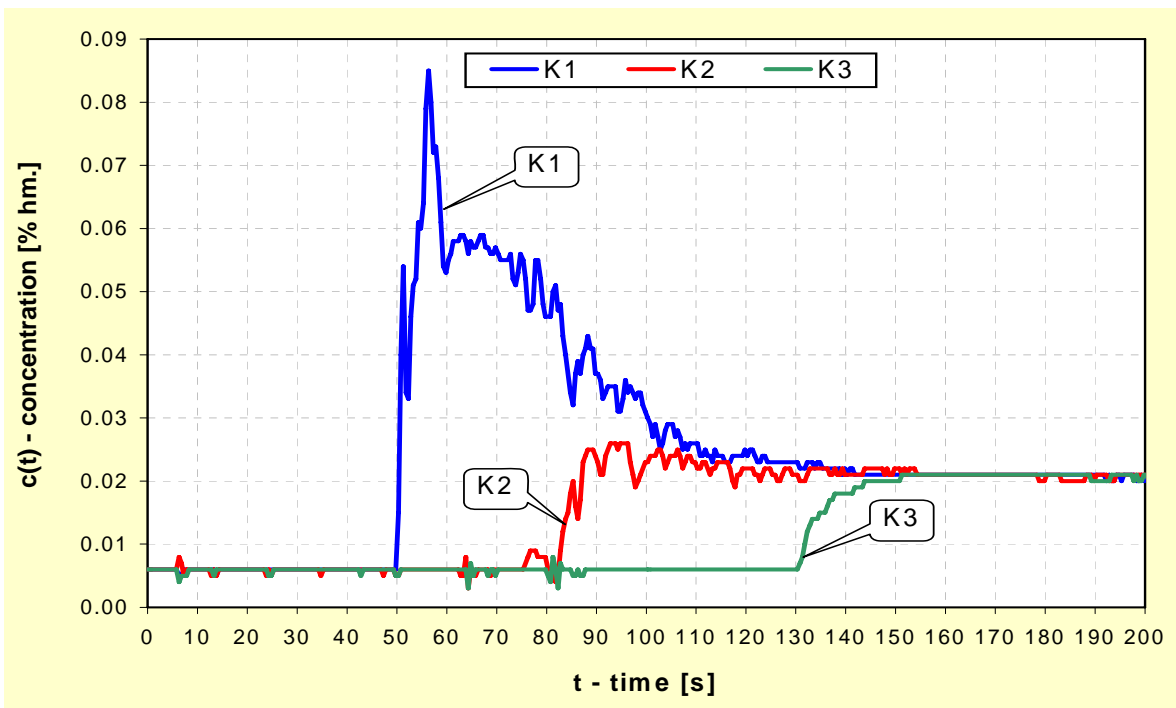Figure 2 – Development of concentration in the sensors *K1*, *K2* and *K3*

Several facts are obvious from the development of concentration in the sensors:

- start and progress of blowing of steel by gas can be approximately considered in the form of the *Heaviside unit step function* and it is therefore possible to consider the development of concentration as *transient characteristics*,
- the sensors reacted only after elapsing of certain "*dead time*", which is proportional to the distance of individual sensors from the liquid level in the *mL*,
- *overshoot* of courses (apparently proportional to the magnitude of the force I or rather to the difference of the forces I and II) also descends with the distance from the liquid level in the *mL*,
- *stable* (final) *value* of concentration is proportional to the proportion of volumes of pure water and water with enriched concentration.

As it can be seen from the *Figure 2*, the initial concentration is not zero, but it corresponds to residual (natural) conductibility of the model liquid (water). For this reason, but also for the needs of comparison of courses in all the sensors, it is appropriate to introduce *standardised* (and dimensionless) concentration according to the following relation:

$$c_n(t) = \frac{c(t) - c_p}{c_u - c_p} \quad [-],$$ (1)

where t – means the time [s],

       $c(t)$ – means the measured concentration [weight %],

       c_p – means the initial value of concentration [weight %],

       c_u – means the stable (final) value of concentration [weight %].

It is obvious from the relation (1), that initial value of the standardised concentration will be *zero* and final (stable) value will be equal to *one*. Due to formation of local concentration heterogeneities in the pool the values of this standardised concentration can during blowing exceed the value of one.

4   Physical – mathematical model

On the basis of the scheme of the *mL* and development of concentrations there was developed simple (based on the principle of the so called Occam's razor: "*entia non sunt multiplicanda praeter necessitatem*" = "models should not be more complex than it is absolutely necessary") *physical-mathematical* model of behaviour of steel concentration in the ladle during its blowing in the form of *cybernetic* model, expressed with use of block diagram in *Figure 3*:
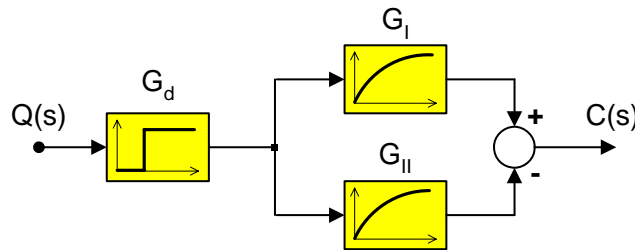

Figure 3 – Block diagram of the ladle model

(the model is valid for any sensor, *Q(s)* is Laplace (L-) image function of gas flow, *C(s)* is L-image of concentration).

Transition of *transport (time) delay* has the following form:

$$G_d(s) \quad = \quad \exp(-T_d \cdot s) \quad = \quad e^{-T_d \cdot s} \quad [-],$$ (2)

where T_d – means the transport delay [s],

       s – means the complex variable in L-transform [1/s].

For the part of the model without *time delay* we therefore presume two parallelly and antagonistically connected *first-order proportional systems* (with transfers G_I and G_{II}), which are used also in (chemical) *kinetics of processes* (in this case, however, in equivalent form of ordinary differential equations of the 1st order with constant coefficients):

$$G_I(s) \quad = \quad \frac{k_1}{T_1 s + 1},$$ (3a)

$$G_{II}(s) \quad = \quad \frac{k_2}{T_2 s + 1},$$ (3b)

where k_1, k_2 – means transfer coefficients of the systems [%·s/m³],

       T_1, T_2 – means time constants of the systems [s].

On the basis of analogy with the so called *subtractional thermocouple* [VÍTEČEK & SMUTNÝ & KUSYN 1988] and on the basis of time behaviour of the measured concentrations (see *Figure 2*) there can be assumed a significant (of an order) difference in the time constant values, i.e. $T_2 \gg T_1$ (that is the descending part of the transient characteristics has considerably bigger time constant than the ascending part), and generally also unequal values of the transfer coefficients $k_1 \neq k_2$.

For this part of the model it is then possible to construct on the basis of algebra of transfers the following continuous L-transfers (for zero initial conditions):

$$G(s) \quad = \quad G_I(s) \quad - \quad G_{II}(s), \tag{4}$$

$$G(s) \quad = \quad \frac{k_1}{T_1 s + 1} - \frac{k_2}{T_2 s + 1} = \frac{(k_1 - k_2) + (k_1 T_2 - k_2 T_1)s}{(T_1 s + 1)(T_2 s + 1)}, \tag{5}$$

from which for the L-image function and original function (obtained by inverse L-transform) *transfer function H(s)* and *h(t)* (response to the Heaviside unit step function of inert gas flow, $Q(s) = 1/s$), as well as for its limit values we get the following:

$$H(s) = C(s) = G(s) \cdot Q(s) = G(s) \cdot \frac{1}{s}, \tag{6}$$

$$h(t) \quad = \quad (k_1 - k_2) - k_1 \cdot \exp(-t/T_1) + k_2 \cdot \exp(-t/T_2), \tag{7}$$

$$h(0) \quad = \quad (k_1 - k_2) - k_1 + k_2 = 0, \qquad h(+\infty) = k_1 - k_2. \tag{8}$$

Due to the fact that the stable value of the *standardised* concentration is equal to one, the following relation is valid for the value of the transfer coefficient k_2 (expressing also the relation that $k_2 < k_1$):

$$h(+\infty) = k_1 - k_2 = 1 \quad \Rightarrow \quad k_2 = k_1 - 1. \tag{9}$$

By insertion of this relation into the relation (7) we get the final expression for the transient function of the standardised concentration, which can be simultaneously used also as non-linear regression model with three parameters k_1, T_1 and T_2:

$$\boxed{h(t) = c_n(t) \quad = \quad 1 - k_1 \cdot \exp(-t/T_1) + (k_1 - 1) \cdot \exp(-t/T_2)}. \tag{F1}$$

To make the image complete let us construct for the L-transform of this part of the system, when after insertion of the obtained relations for the transfer coefficient into the relation (5), we get the following:

$$G(s) \quad = \quad \frac{\{k(T_2 - T_1) + T_1\}s + 1}{(T_1 s + 1)(T_2 s + 1)}, \tag{10a}$$

$$G(s) \quad = \quad \frac{T_D s + 1}{(T_1 s + 1)(T_2 s + 1)}, \quad T_D = f(k, T_1, T_2), \tag{10b}$$

$$T_D = k(T_2 - T_1) + T_1, \tag{10c}$$

from which it is evident that this is a modification of the so called real *derivative element* with lag of the 2nd order, whereas the derivation time constant T_D is function of all three parameters. This transfer (and thus also behaviour of the model) corresponds even better to the transfer of the real *PD regulator*, but with mutually different real poles (classical real PD regulator has two conjugate complex poles) – see [KUBÍK et al. 1974].

The model *F1* can be obtained also by another way, by logical thinking. It is possible to

construct the curves of similar type from exponentials or to use *equations of chemical kinetics* (which can be almost or completely the same). The simplest way is summation of two exponentials (ascending and descending) and the constant:

$$c(t) \;=\; a_1\{1-\exp(-a_2 t)\}+a_3\cdot\exp(-a_4 t)+a_5, \tag{11}$$

which leads at conditions c(0) = 0, c(∞) = 1 and after formal assignment of $b_1 = a_1$, $b_2 = a_2$, $b_3 = a_4$, to the regression equation (F1m), corresponding to the model *F1*, whereas the following equivalence is valid for its coefficients $b_1 = k_1$, $b_2 = 1/T_1$ [1/s], $b_3 = 1/T_2$ [1/s]:

$$\boxed{c_n(t) \;=\; 1-b_1\cdot\exp(-b_2 t)+(b_1-1)\cdot\exp(-b_3 t)}. \tag{F1m}$$

Coefficients b_2 and b_3 have at the same time in this equation a character of kind of velocity or frequency constants of mixing process.

5 Simulation model and its identification

Simulation identification of the part of the model with transfer *G(s)* (see the relation (4)) was realised in the simulation software *20-sim 2.3 Pro* (shareware, University of Twente, The Netherlands, 1998, www.20sim.com) [ZÍTEK & PETROVÁ 1996], according to the diagram (*argon2.mg0*) – see *Figure 4*:
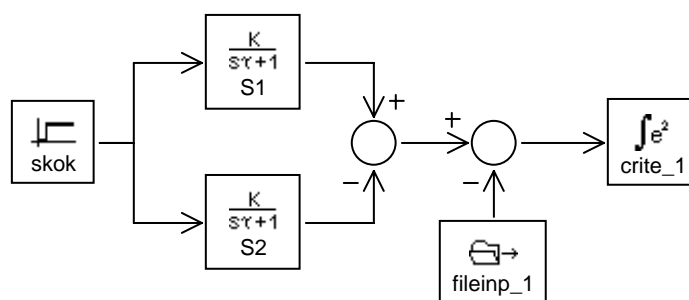

Figure 4 – Simulation diagram of the ladle model in the program *20-sim*

Identification of a continuous *mL* was realised for the following settings and values of the *simulation* parameters:
- initial setting $k_1 = 5$, $T_1 = 5$ s, $T_2 = 50$ s,
- optimisation method Broydon-Fletcher-Goldfarb-Shanno,
- tolerance = 0.01,
- integration method *RK4* (Runge-Kutta of the 4th order),
- integration step $h = 0.5$ s (corresponding to the period of data reading),
- final time of simulation *tf* = 160.5 s,
- ranges (limits of values) of parameters: $k_1 \in <1, 10>$, $T_1, T_2 \in <1, 100>$.

Results of simulation parametric identification (with use of optimisation criterion ISE = Integral of Squared Error) from the simulation program *20-sim 2.3 Pro* for the data set *LP_K1n.dat*, i.e. data of standardised concentration $c_{n1}(t)$ in the 1st sensor *K1*, are summarised in the *Table 1*:

Table 1. Results of simulation parametric identification for the data *LP_K1n*

k_1	T_1	T_2	ISE	Note
6.247	3.237	26.598	8.748	h = Δt = 0.5 s

Figure 5 shows courses of the values *y* (model output) and *ys* (output form the system, i.e. measured and standardised data) for concentration from the sensor *K1* (*argon3.mf3*, experiment *exp1*):
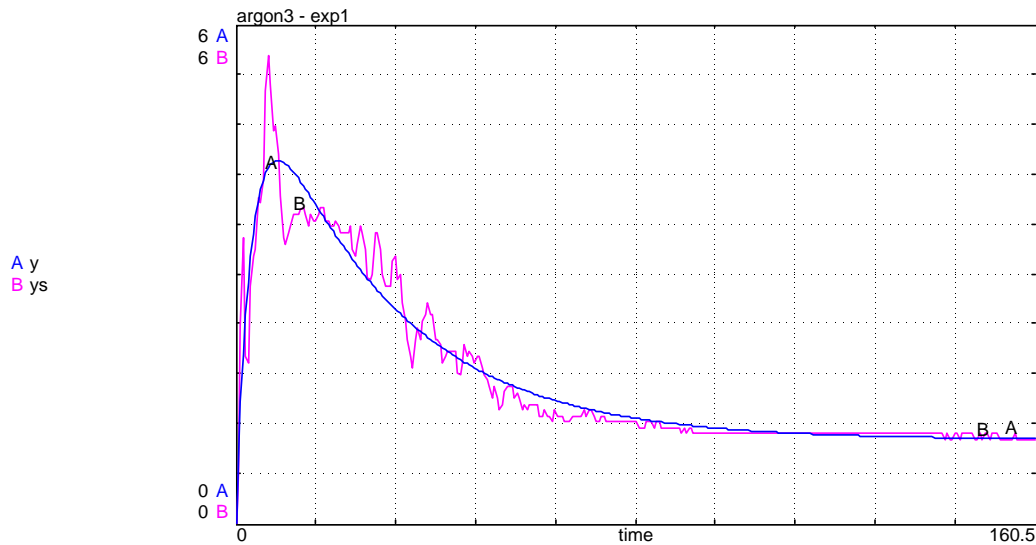

Figure 5 – Courses of the values in the program *20-sim* (for data *LP_K1n.dat*)

It is evident from the *Figure 5*, that simulation identification provided acceptable results – regression course of the output from the approximation system (model) corresponds quite well with the measured values of the standardised concentration.

Similarly acceptable results were obtained by simulation identification also for the concentrations measured in the sensors *K2* and *K3*.

6   Empirical mathematical models

Apart from the obtained *physically adequate* mathematic (and corresponding regression) model *F1*, or modified model *F1m*, there were developed also three *empirical* models (called also empirical formulas, functions or relations) – types and principles of their selection are described e.g. in [BRONŠTEJN & SEMENĎAJEV 1964], [PECHOČ 1981], [KROPÁČ 1987].

The difference between both types of models consists in the fact, that *physically adequate* model (called also theoretical, deterministic or phenomenological model) corresponds (although often in a simplified manner) to physical laws, its parameters have physical meaning and can be therefore used also for extrapolation of the measured values.

Empirical mathematical (regression) models generally do not have these properties and „try" only to express in the best possible way the courses (trends) in data, whereas their use is correct only for interpolation of the values (within the interval of independent variable).

Empirical models, fulfilling the *marginal conditions* $c_n(t = 0) = 0$, $c_n(t \to +\infty) = 1$, for the standardised concentrations have the following form:

$$c_n(t) \quad = \quad \frac{t^{b_1} - b_2}{b_2 + b_3 \cdot t^{b_4}} + 1, \tag{E1}$$

$$c_n(t) \quad = \quad \frac{b_1 t + b_2 t^2 + b_3 t^3}{1 + b_4 t + b_5 t^2 + b_3 t^3}. \tag{E2}$$

Both empirical functions have the form of *rational polynomial (ratio of power functions)*, whereas the model *E1* has 4 parameters and model *E2* even 5 parameters.

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Another possibility is an empirical model constructed as summation of two functions: *Hoerl' function* (f₁) and suitable multiple of the *function arc tangent* (f₂), whereas the following is valid for their marginal values: $f_1(0) = f_2(0) = 0$, $f_1(\infty) = 0$, $f_2(\infty) = 1$:

$$c_n(t) \;=\; b_1 \cdot t^{b_2} \cdot \exp(-b_3 t) + \frac{2}{\pi} \cdot arctg(b_4 t).$$
(E3)

The mentioned empirical mathematical models can be characterised (from cybernetic viewpoint) as so called *grey boxes*, i.e. there were known not only inputs and outputs, but also additional (subsidiary) conditions [KROPÁČ 1987] in the form of the marginal conditions referred to above.

7 Comparison of models

For the data *LP_K1n.dat* of standardised concentration measured in the sensor *K1*, there were compared the results obtained for four models, namely:
- with use of the above mentioned *simulation identification* (only in physically adequate model, hereinafter marked as *F1s*),
- and also with use of *non-linear regression* (on all four model).

The results are summarised in the *Table 2* (where criterion SSE = *S*um of *S*quared *E*rror) - and for non-linear regression also in the *Figure 6*:

Table 2. Results of identification and non-linear regression for data *LP_K1n*

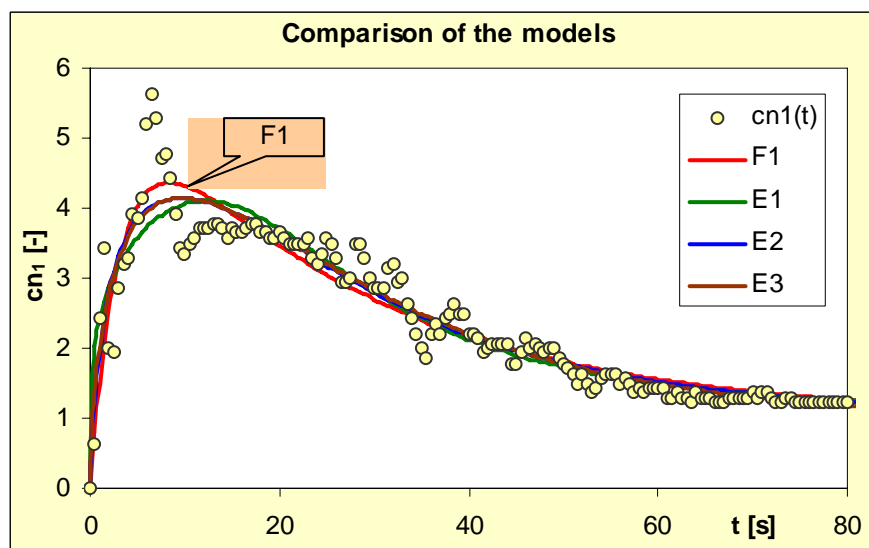| Model	k_1 b_1	T_1 b_2	T_2 b_3	b_4	b_5	ISE SSE	R^2 [%]	Note
F1s	6.247	3.237	26.598	-	-	8.75	-	h = 0.5 s
F1	6.238	3.214	26.633	-	-	19.33	94.12	*3 parameters*
E1	0.252	0.416	0.000057	2.751	-	22.15	93.26	4 –,,–
E2	3.058	-0.023	0.00062	0.578	*-0.0041*	18.42	94.40	5 –,,–
E2r	2.791	-0.018	0.00050	0.490	-	18.48	94.38	4 –,,–
E3	1.743	0.512	0.0558	*0.605*	-	17.92	94.55	4 –,,–

Figure 6 – Comparison of the models for the data *LP_K1n.dat*

It is obvious from the comparison that:
- *simulation identification* and *non-linear regression* give for physically adequate model

F1 practically the same results (which could have been expected due to similar optimality criterion),

- the models are qualitatively comparable (with respect to the „integral" quality of approximation, expressed by the indicators R^2 and SSE),
- in spite of the fact that in empirical model *E2* there has occurred within the interval of time values of approx. 131.5 to 10^8 seconds an „undershoot" below the value 1 and the coefficient b_5 is statistically insignificant, which means that the following modified and reduced model with 4 parameters would be sufficient:

$$c_n(t) \quad = \quad \frac{b_1 t + b_2 t^2 + b_3 t^3}{1 + b_4 t + b_3 t^3}, \tag{E2r}$$

as all its coefficients are already statistically significant and determination coefficient R^2 was here decreased only by 0.02 %,

- similarly in the empirical model *E3*, which has practically identical course as the model *E2*, there has occurred within the interval of time values of approx. 144 to 10^7 seconds an „undershoot" below the value 1 and the coefficient b_4 is statistically insignificant (however, in this model it cannot be deleted),
- nevertheless *the best* is the model *F1*, which is physically adequate, has the smallest number of parameters and at ascending part it provides adequate growth of the values (empirical model *E1* has here a too steep growth).

8 Regression model in all concentrations

The *Table 3* and the next *Figure 7* show visible use of the model *F1* for standardised values of concentration in all three sensors (without considered *time delay*):

Table 3. Results of non-linear regression for the model *F1*

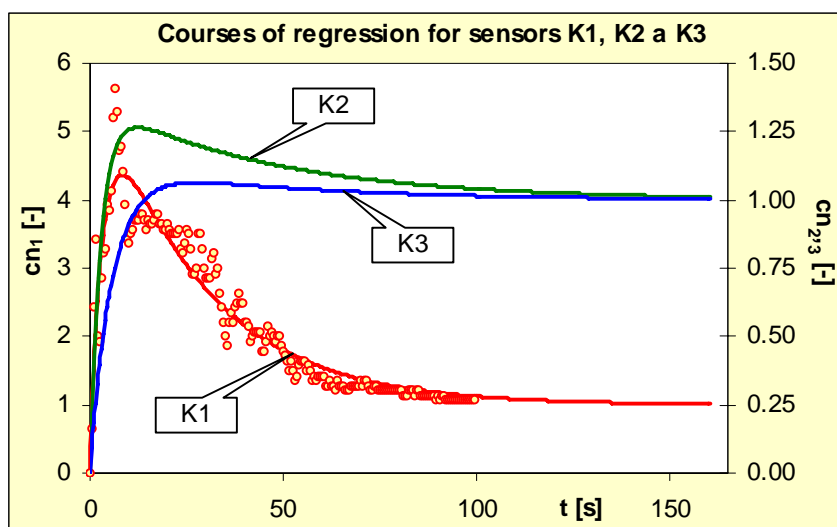| Sensor	k_1 [%·s/m³]	T_1 [s]	T_2 [s]	R^2 [%]	Note
K1	6.2	3.2	26.6	94.12	
K2	1.4	2.9	45.1	74.98	min. R^2
K3	1.1	5.7	46.5	96.62	max. R^2

Figure 7 – Courses of regression of the model *F1* for the data from all three sensors

It is evident from the results that the model *F1* is suitable and usable for description of the development of concentration in all three sensors. It is also obvious that the transfer coefficient (gain coefficient) k_1 decreases with the distance of the sensor from the liquid level in the *mL*, while the time constant T_2 increases in this dependence.

9   Use of the model for evaluation of experiments

It is apparent that the proposed *physically adequate model* can be used for evaluation of results of physical modelling of processes at blowing of steel in the ladle model. In the series (of approx. 120) experiments realised in *the laboratory of physical modelling* at the *Třinec steelworks, a.s.* some basic values of simulation were being changed, namely:

- q – volume flow of the blown argon,
- e – eccentricity, position of the blowing elements,
- n – number of the blowing elements.
  It is generally possible to change also:
- V – volume of the pool in the ladle model,
- ρ – density of the „top" and „bottom" layer of the pool (ρ_h, ρ_s)
- c – and their concentration (c_h, c_s).

Concentration was in the course of measurement moreover read in three sensors $c_i(t)$, index $i \in \{1,2,3\}$, which must also be taken into consideration.

It follows from the above facts that the parameters or „*constants*" of physically adequate model T_d, k_1, T_1 and T_2 are in fact *functions* of the simulation input parameters, i.e. the following is valid:

$$T_d = T_d(V, \rho_h, \rho_s, c_h, c_s, q, e, n, i) \text{ etc.}$$

Thanks to standardisation of concentrations (c_h, c_s), use of the same pool (ρ_h, ρ_s) of the same volume (V), as well as one blowing element ($n = 1$) in the certain position (e) it can be presumed that the model parameters would be functions of the small set of (in fact two) pars of simulation, i.e. that the following would be valid:

$$T_d = T_d(q, i).$$

Assessment of dependences of the model parameters on the input parameters of the realised simulations, however, could and should already be the subject of another separate paper.

10 Conclusion

For the description of measured concentrations changes of the bath elements in the ladle model there were developed and verified four mathematical (regression) models, namely one *physically adequate* and three *empirical*.

Out of these models the most suitable and at the same time the most simple (which corresponds to the principle of the so called Occam's razor: „the simplest is usually correct or at least suitable") was the *physically adequate model*, which can be (and also was) used for the next analysis of influence of simulation input parameters on coefficients of this model, both for setting of suitable (optimum) mode of operation at blowing of steel in the ladle.

Didactical usability of the contents of this paper is also not negligible, as it can be used for teaching at (not only technical) universities.

11 References

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