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Volume 3 includes abstracts of plenary lectures of Congress, keynote lectures, invited reports, oral and poster presentations, and correspondent presentations of the sections: “Physical chemistry of metallurgical processes”, “Topical problems of chemical industry, evaluation of technical risks”, “Chemical aspects of alternative energetics” and author index..

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CRITERION DAMKOHLER AS PARAMETER DEFINING MATHEMATICAL DESCRIPTION OF NON-STATIONARY OPERATING MODES OF CSTR

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The system of "continuous stirred tank reactor (CSTR) + reaction" is interpreted as dynamic link of 2nd order, like the transducer and regulator. In the case of reaction $A_1 \xrightarrow[n_1]{k_1} \alpha_2 A_2 \xrightarrow[n_2]{k_2} \alpha_3 A_3$ linearized mathematical model has the following form at the action of various destabilizing factors (DF)[1]

$$\varepsilon_2'' + (A_1 + A_2)\varepsilon_2' + A_1 A_2 \varepsilon_2 = f_{\mathrm{DF}}(\overline{\tau}), \qquad \textbf{(1)}$$

where $|\varepsilon_2| = |c_2 / c_{02} - 1| << 1$ – is the relative deviation of the concentration c_2 of product A_2 from the nominal value c_{02}; $f_{\mathrm{DF}}(\overline{\tau})$ – is the function defined by the view of DF: $f_{\mathrm{DF}(c)} = n_1 \tilde{A}_1 \tilde{A}_2 \varepsilon_1^{\mathrm{inl}}(\overline{\tau})$ at perturbation $\varepsilon_1^{\mathrm{inl}}(\overline{\tau}) = c_1^{\mathrm{inl}} - 1$ of reagent A_1 concentration c_1^{inl} on inlet of CSTR, $f_{\mathrm{DF}(v)} = a\varepsilon_v(\overline{\tau}) - \varepsilon_v'(\overline{\tau})$ at perturbation $\varepsilon_v(\overline{\tau}) = v / v_0 - 1$ of the volumetric flow rate v, $f_{\mathrm{DF}(k_{\mathrm{d}})} = f(A_i, \tilde{a}_2, \overline{k}_{\mathrm{d}(i)}, \overline{\tau})$ at low catalyst deactivation with constants $\overline{k}_{\mathrm{d}(i)} \propto k_{\mathrm{d}(i)}\tau_0$ deactivation of reaction stages; $\overline{\tau} = \tau / \tau_0$ – is the time in units of mean residence time τ_0.

The constants A_i and $\tilde{A}_i$ in the equation (1) are the conversion coefficients (CC) of subsystems "CSTR + *i*-th stage"

$$A_i = 1 + n_i \tilde{a}_i,\ \tilde{A}_i = 1 + \tilde{a}_i,\ \tilde{a}_i = n_i^{-1} \partial \overline{w}_{0i} / \partial c_{0i} = k_{0i}\tau_0 C_{0i}^{n_i - 1} \equiv \mathrm{Da}_{0i}, \qquad \textbf{(2)}$$

i.e. the first criterion Damkohler[2] Da_{0i} is equal to the sensitivity of reaction rate $\overline{w}_{0i}$ to quasi-stationary changes of c_{0i} or synonymously is equal to CC of the reaction in reactor: $\mathrm{Da}_{0i} \propto k_{0i}\tau_0$ (for CSTR as apparatus $\tilde{a}_{\text{r-or}} = \mathrm{Da}_{\text{r-or}} \equiv 1$).

The magnitudes Da_{0i} are determined by the degree of transformation $x_0(\tau_0) = 1 - \tilde{n}_{01}$ of A_1 and by the selectivity $s_{02}(x_0) = 1 - s_{03}$ of the A_3 product formation process

$$\mathrm{Da}_{01} = x_0 / c_0,\ \mathrm{Da}_{02} = s_{03} / s_{02}, \qquad \textbf{(3)}$$

i.e. they are determined by the simplexes[3] $y_0 \equiv x_0 / c_0$ and $z_0 \equiv s_{02} / s_{03}$.

References

1. Lucheyko I.D. *IV International Conference on Chemistry and Chemical Technology,* 2015, Erevan, 242.
2. Carl W. Hall. Laws and Models: Science, Engineering, and Technology. CRC Press, 1999.
3. Lucheyko I.D. *Nauk. visti NTUU "KPI"*, 2012, **6**, 145.

Leontiev L.I. **123**, **199**, **208**, **212**
Levashov E.A. **77**
Lindhorst T.K. **20**
Lipilin A.S. **359**
Lisienko D.G. **201**
Litvinova I.S. **49**
Litvinov B.V. **120**
Lobanov A.V. **346**
Loginova I.V. **220**
Lokshin E.P. **168**, **169**
Lomakin G.V. **280**
Lubchenko N.P. **358**
Lubnin A.N. **166**
Lucheyko I.D. **298**, **299**
Lucheyko I.I. **308**
Luchneva S.I. **170**
Lukanin P.V. **338**
Lyadov A.S. **253**
Lyagaeva J.G. **347**
Lykasov A.A. **136**
Lypenko D.A. **377**, **378**
Lysakova T.P. **377**, **378**
Lysak V.I. **33**, **144**, **164**

M

Magomedova A.O. **219**
Maiorova A.V. **274**
Makarenkov D.A. **437**
Makarova A.S. **254**
Makarova I. **335**
Makarova N.I. **377**
Makarov A.V. **78**
Makhin M.N. **204**
Makhonina E.V. **348**
Makrovets L.A. **81**, **171**
Maksimov A.L. **386**
Maleeva M.A. **134**
Maltseva I.E. **155**
Maltsev E.I. **377**, **378**
Malyshkin D.A. **325**, **364**
Malyutin L.N. **172**
Mamyachenkov S.V. **133**
Manaenkov O.V. **416**
Mansurova A.N. **173**, **196**
Marchenkova E.B. **132**
Marchenkov V.V. **132**
Markov A.A. **240**
Markushev M.V. **72**
Maslennikov A.N. **118**, **204**
Mastyugin S.A. **79**
Matushkina A.N. **112**
Matveenko L.A. **365**
Matveeva V.G. **416**, **444**
Mavlyudova Ya.A. **437**
Medvedeva A.E. **348**
Medvedev D.A. ... **314**, **329**, **347**, **352**, **400**, **408**
Medyankina I.S. **174**, **182**, **188**
Melchakov S.Yu. **201**
Melekh B.T. **376**
Melentyev A.B. **296**
Melikhov I.V. **396**
Melkomukova O.G. **175**
Melkonyan R.G. **255**
Melnichenko E.I. **80**, **176**
Menshikov S.Yu. **240**, **275**
Meshalkin V.P. **233**, **241**, **276**, **300**
Meshcheryakova M.O. **319**
Meshcheryakova Y.V. **438**, **439**
Meylakh A.G. **70**
Mikhailov G.G. **81**, **109**
Mikheykin A. **335**
Miller J.S. **21**
Miluytina A.D. **297**
Minaev Y.A. **55**
Mindubaev A.Z. **277**
Minkin V.I. **377**
Miroshnichenko M.N. **68**, **153**
Miroshnikov A.I. **22**
Mishchenko E.V. **302**
Misin V.M. **248**
Mitu B. **341**
Mizina L.V. **157**, **158**, **162**
Modestov A.D. **429**
Mohri T. **38**
Mordanov S.V. **296**
Morozov A.A **431**
Morozov A.E. **51**
Moshev E.R. **241**
Mukhamed'yarova A.N. **256**
Muradymov R.V. **368**
Mushnikov P.N. **320**, **362**, **401**
Muzhdabaeva M.A. **137**

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