A KINETIC MODEL OF COAL LASER PYROLYSIS

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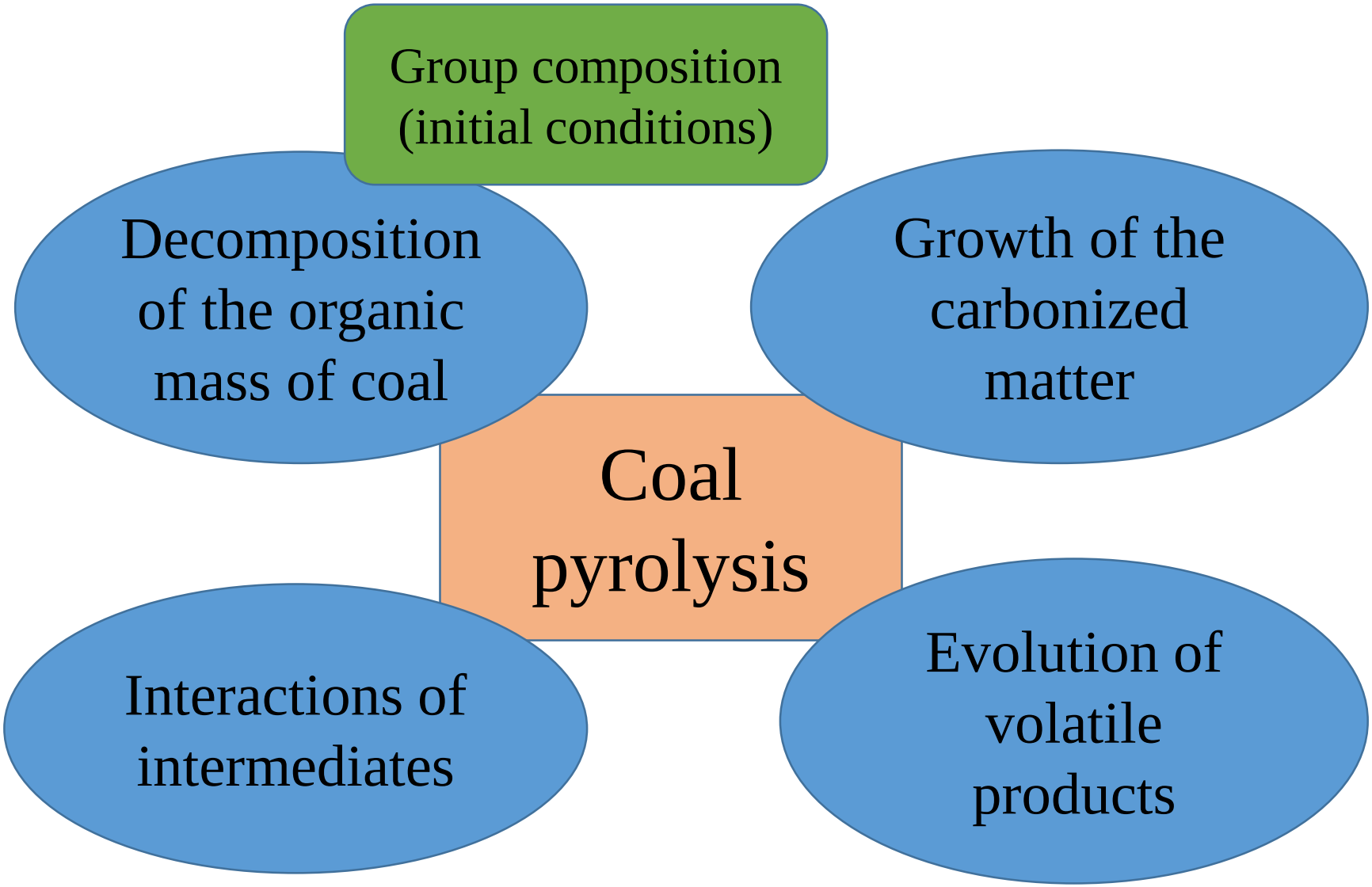
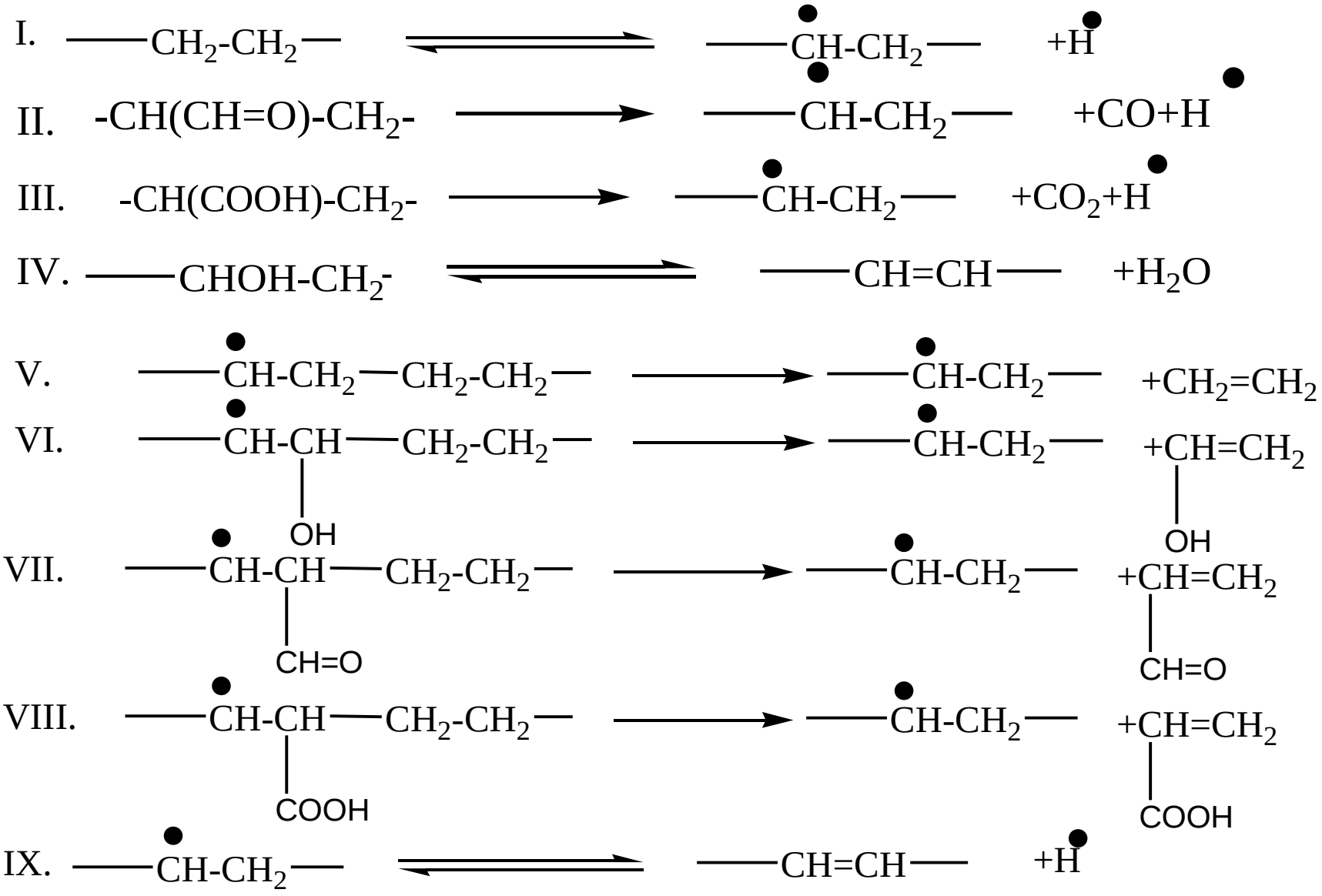
Motivation

- The laser pyrolysis is a physical model of processes occur when a coal particle enters a swirl furnace heating the particle due to the wall's incandescence.
- The pulse heating is able to shift the ratios of the characteristic rates of the organic mass of coal destruction that, in turn, may lead to the changes in the pyrolysis products.
- Similar processes could be observed in the case of laser pyrolysis of various organic substances.

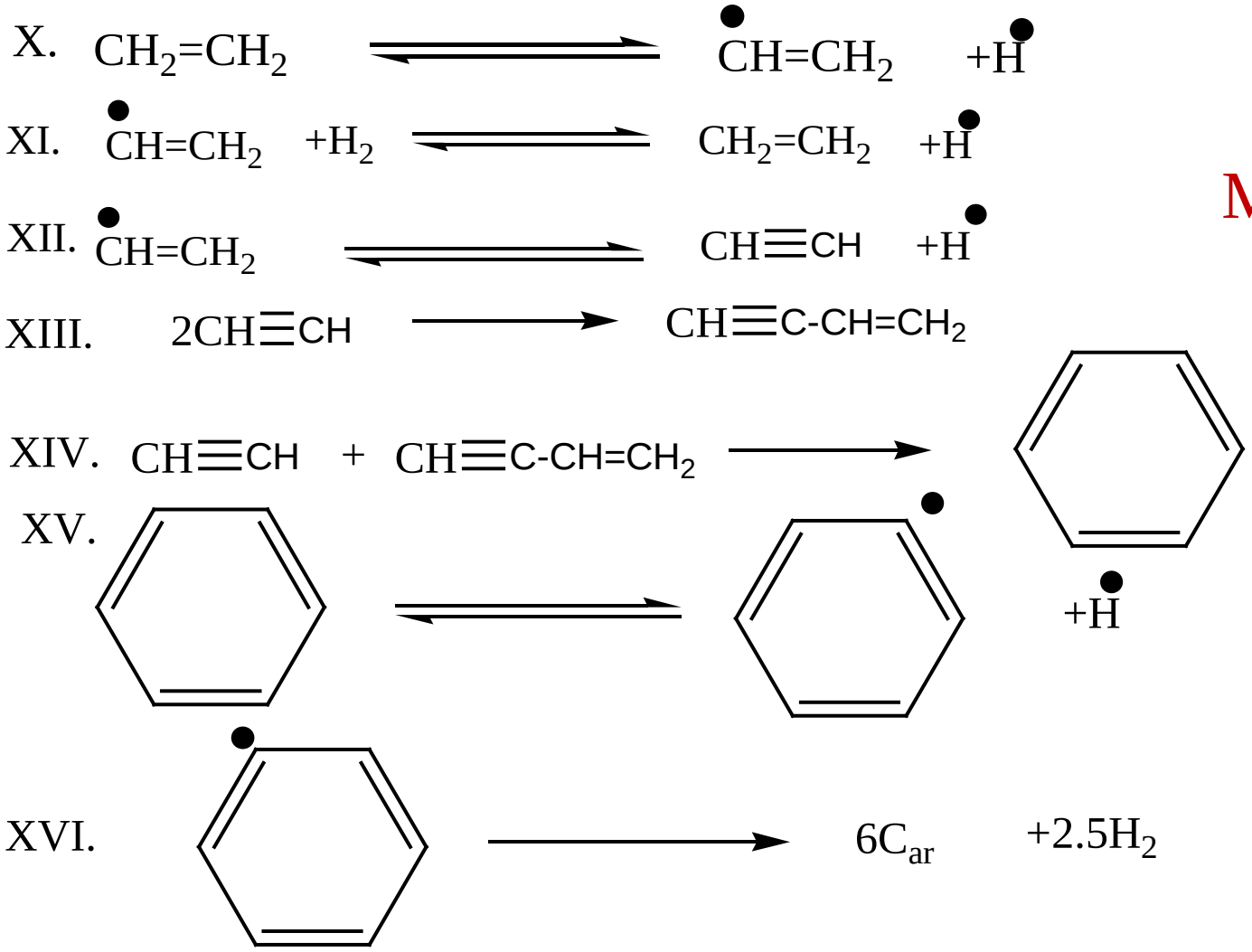
The **objective** of the present work is the development and primary analysis of the coal pyrolysis model initiated with laser pulses of submicrosecond duration.


Group composition
(initial conditions)
Decomposition
of the organic
mass of coal
Growth of the
carbonized
matter
Coal
pyrolysis
Interactions of
intermediates
Evolution of
volatile
products

Decomposition of the organic mass



Growth of the carbonized matter

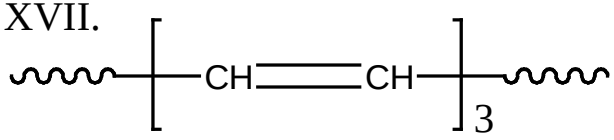


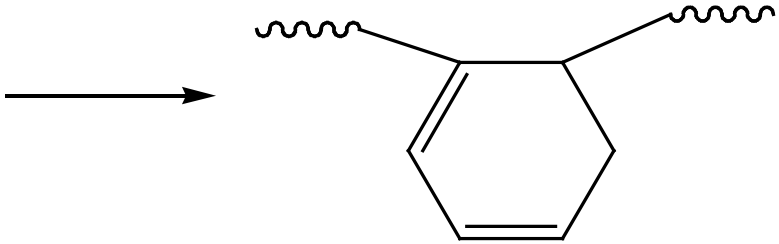
Mechanism I

Growth of the carbonized matter

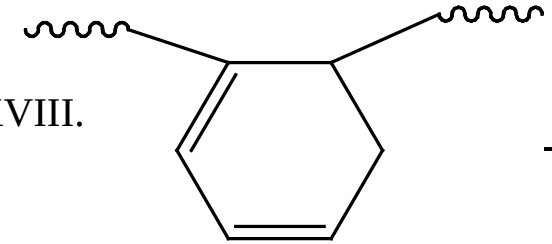
Mechanism II

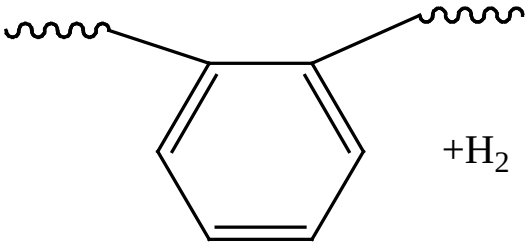
XVII.





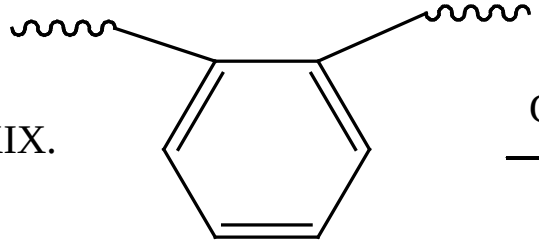
XVIII.





$+H_2$

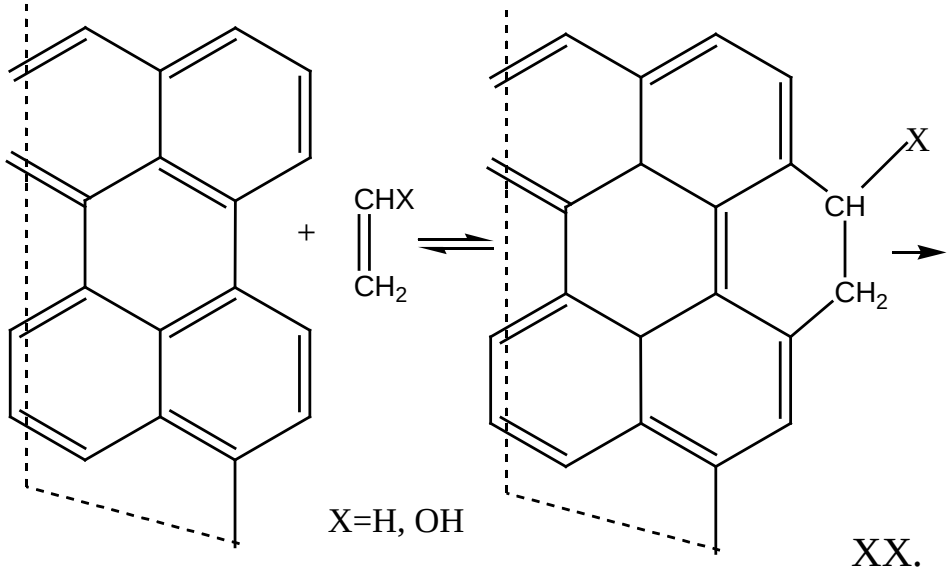
XIX.



$C_{arom\ core}$

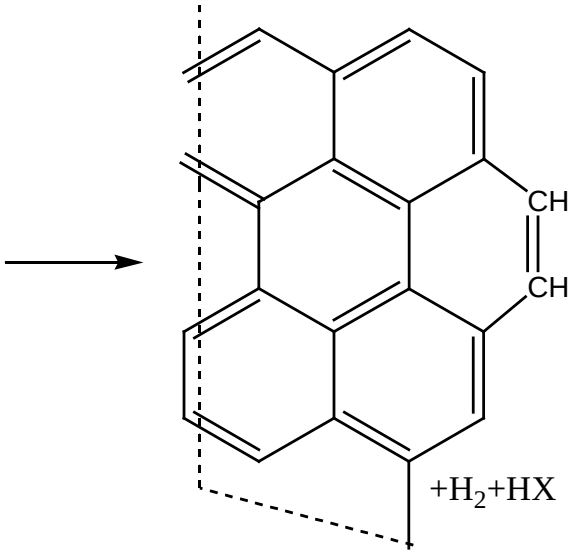
$6C_{ar}$ $+2H_2$

Growth of the carbonized matter



Mechanism III

XX. $CH_2{=}CH_2 \xrightarrow{C\ \text{arom core}} 2C_{ar} + 2H_2$

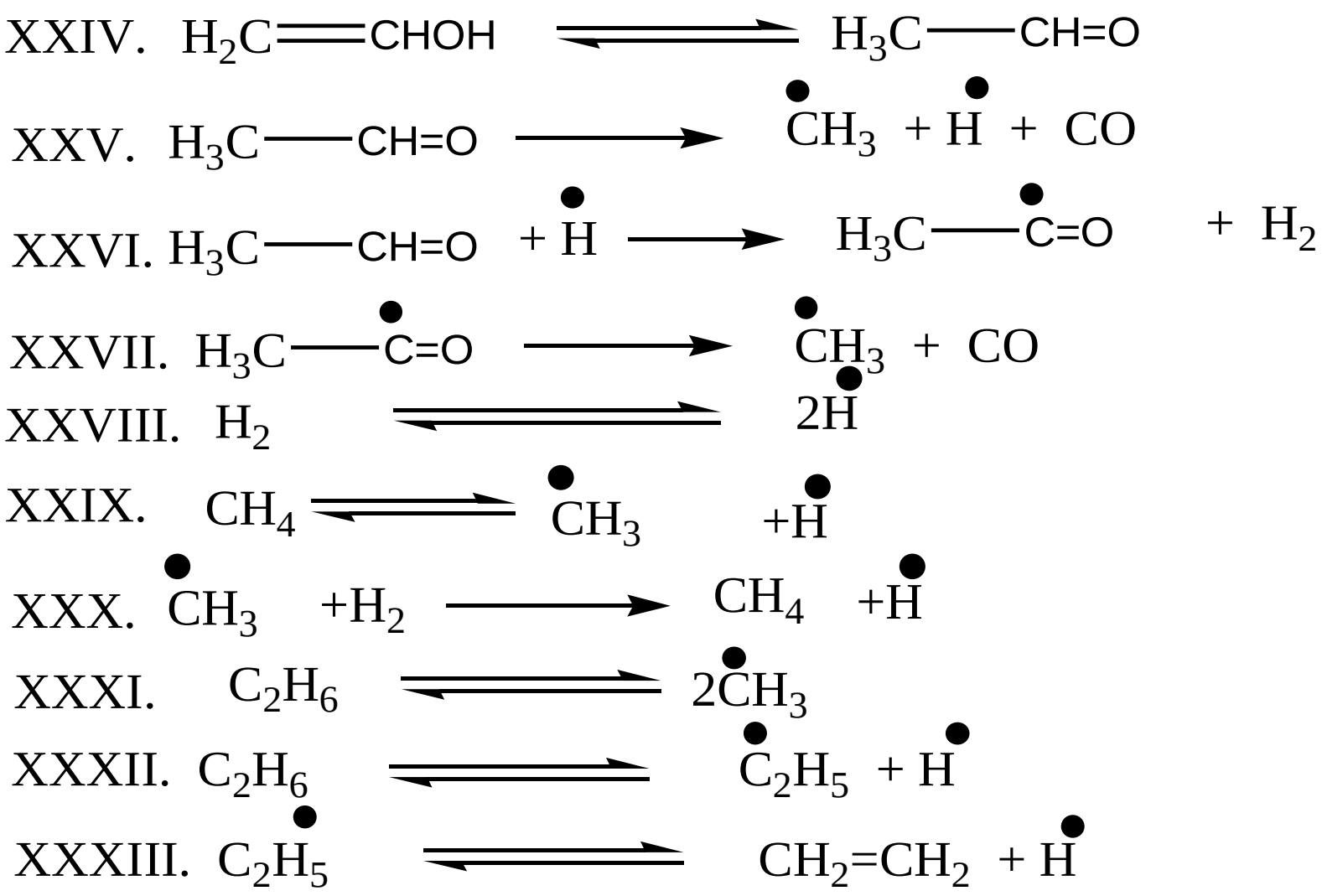


XXI. $CH_2{=}CH{-}OH \xrightarrow{C\ \text{arom core}} 2C_{ar} + H_2 + H_2O$

XXII. $CH_2{=}CH{-}CH{=}O \xrightarrow{C\ \text{arom core}} 2C_{ar} + 2H_2 + CO$

XXIII. $CH_2{=}CH{-}COOH \xrightarrow{C\ \text{arom core}} 2C_{ar} + 2H_2 + CO_2$

Interactions of intermediates



Initial conditions

- On the base of the elemental composition

$$n_C = \frac{\pi}{4} \cdot \left(\frac{L_a}{l} \right)^2$$

$$n_H = \frac{4}{3} \sqrt{\pi n_C}$$

$$\begin{pmatrix} [C_{Ar}]_0 \\ [-CH_2 - CH_2 -]_0 \\ [-CH_2 - CHOH -]_0 \end{pmatrix} = (1 - A^d) \cdot (1 - W^a) N_A \cdot \begin{bmatrix} n_C & 2 & 2 \\ n_H & 4 & 4 \\ 0 & 0 & 1 \end{bmatrix}^{-1} \begin{pmatrix} 12C^{daf} \\ 1H^{daf} \\ 16O^{daf} \end{pmatrix}$$

- Using C13 NMR results

$$\omega_C = \omega_C^{daf} \cdot (1 - W) \cdot (1 - A^d)$$

$$[Ar]_0 = \frac{\rho \cdot \omega_C \cdot X_{Ar} \cdot N_A}{M_C \cdot N_{Ar}}$$

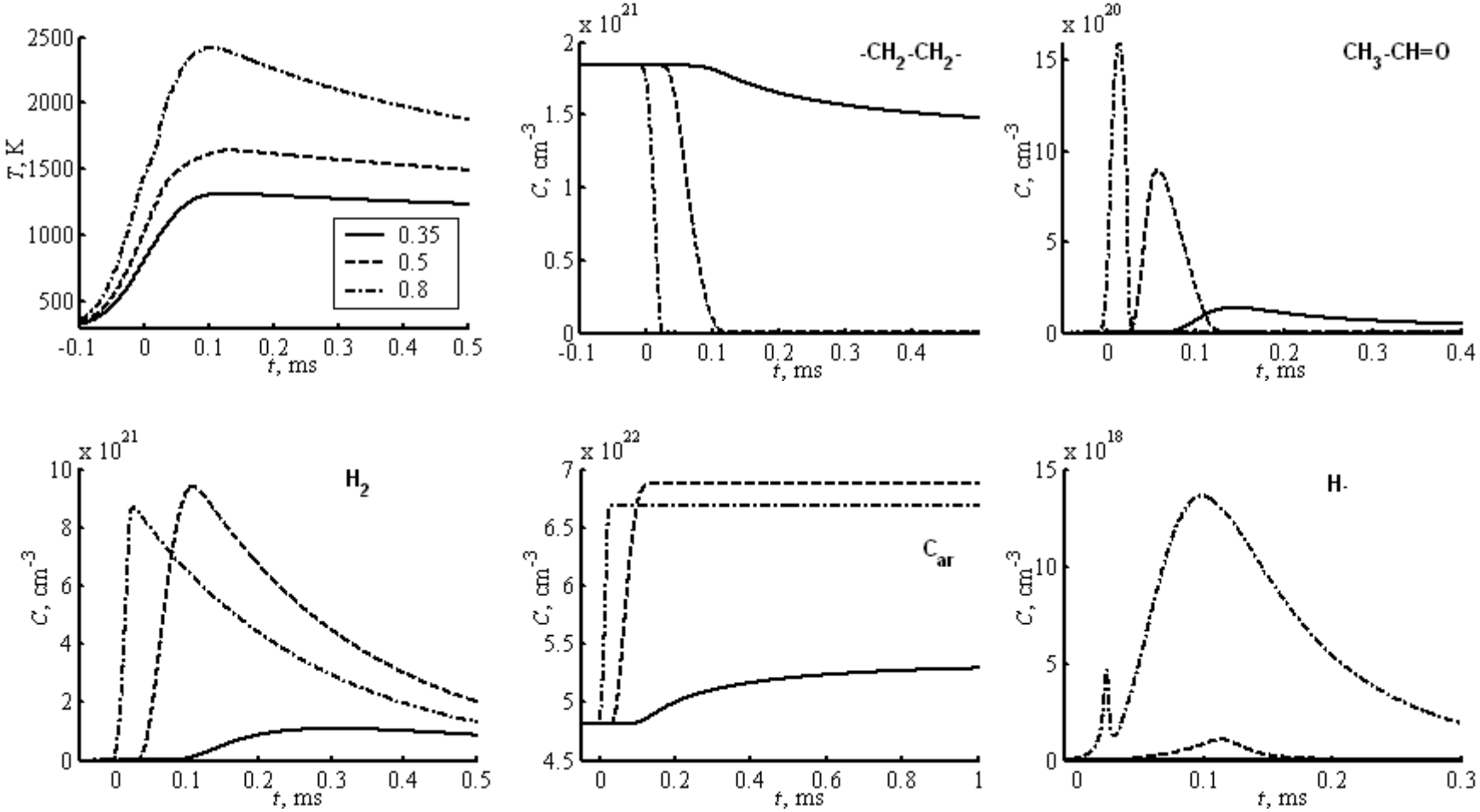
$$[i]_0 = \frac{\rho \cdot \omega_C \cdot X_i \cdot N_A}{M_C}$$

Tisul lignite

C=O	COOH	C_{ar}-O	C_{ar}	C O_{alk}-O	C_{alk}-O	C_{alk}
4.4	4.7	4.2	19.1	3.5	7.5	55.6

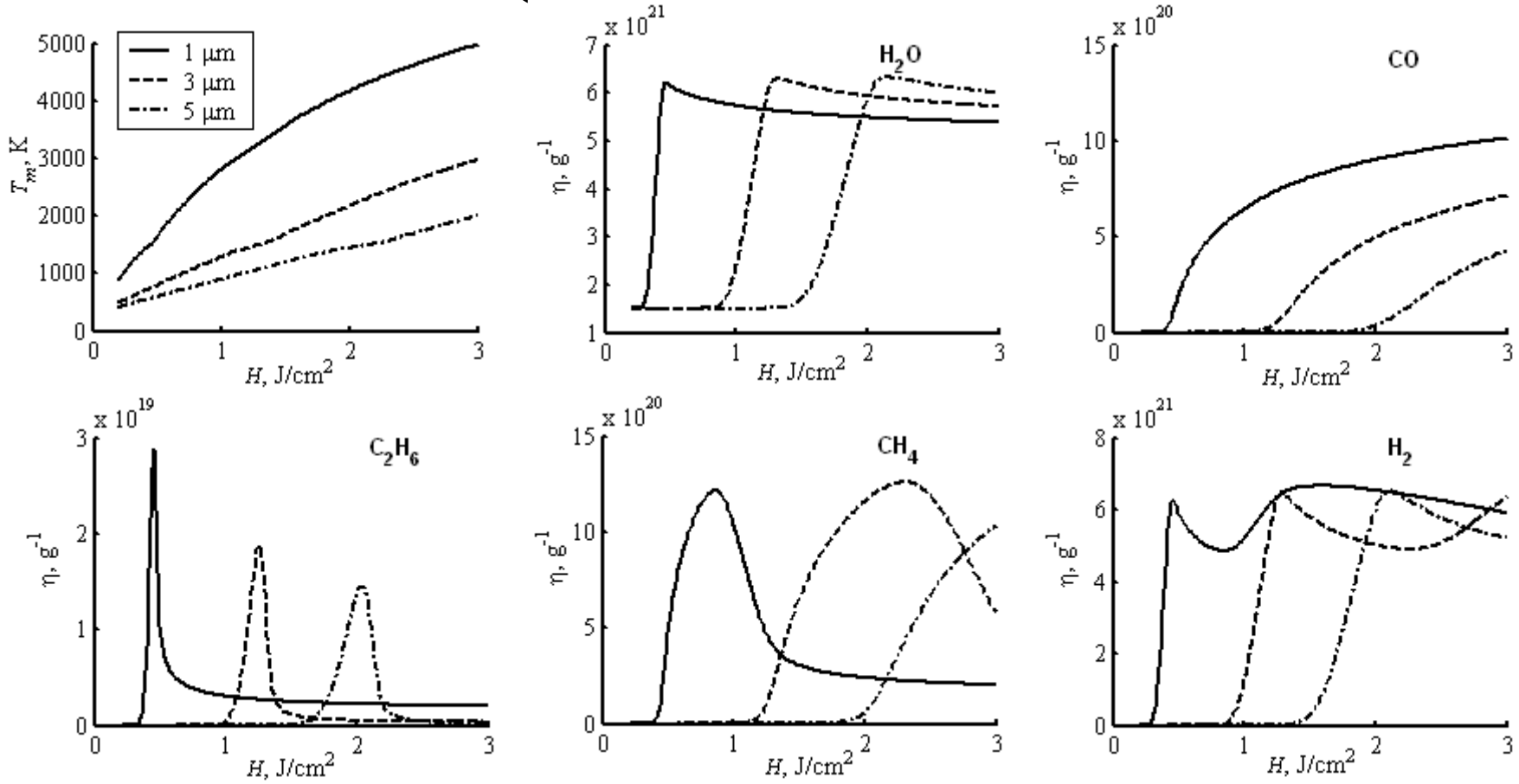
-CH_2-CH_2-	-CHOH-CH_2-	-CH_2-CH(-CH=O)-	-CH_2-CH(-COOH)-	H_2O
6.992	5.827	2.331	2.490	5.111

Results (sub-bituminous coal)



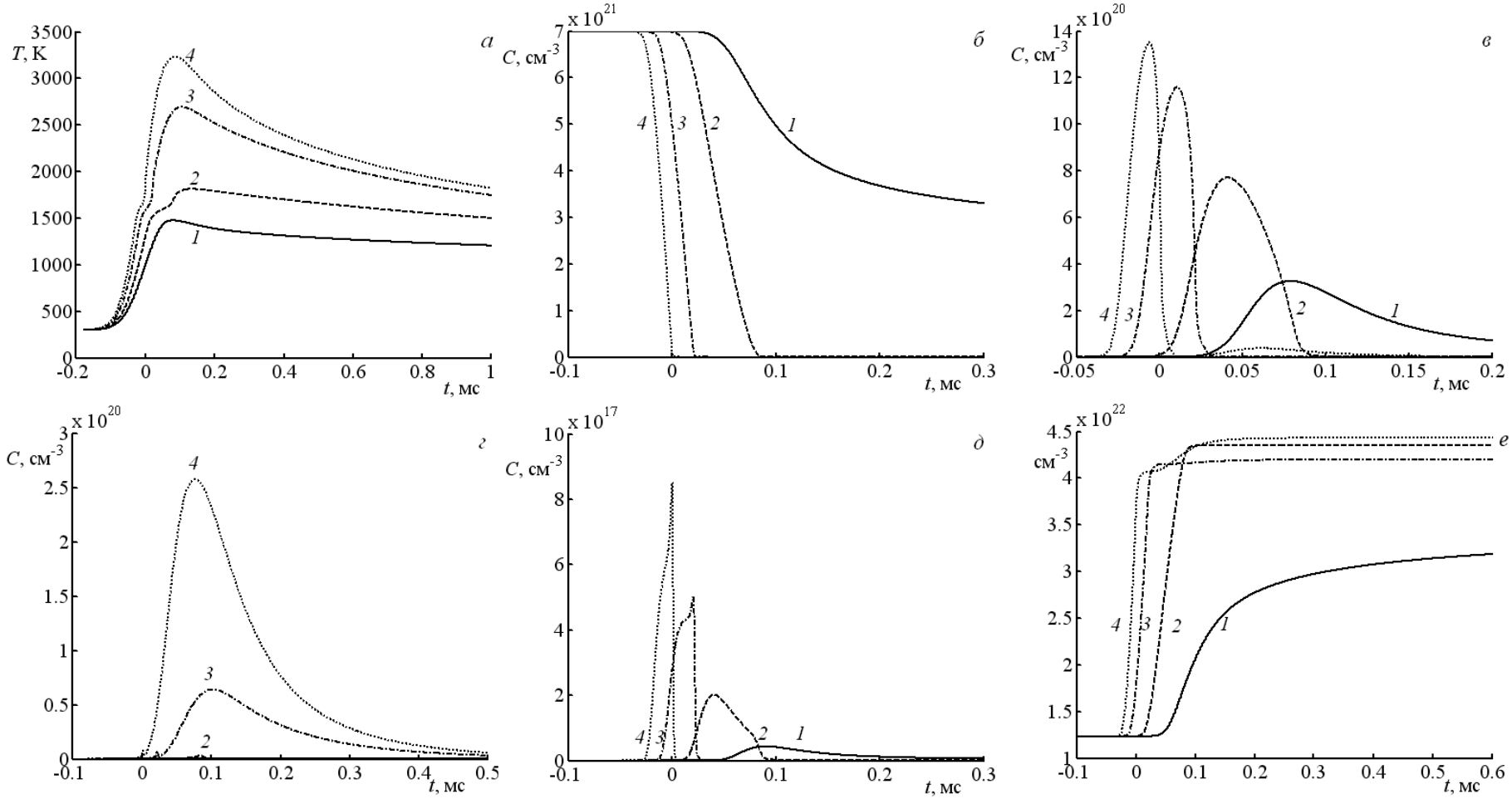
The calculated kinetiks of temperature and reagents' concentrations during laser pulse pyrolysis of subbitumenous coal particles with effective radius 1 μm and energy density values 0.35, 0.5, and 0.8 J/cm^2.

Results (sub-bituminous coal)



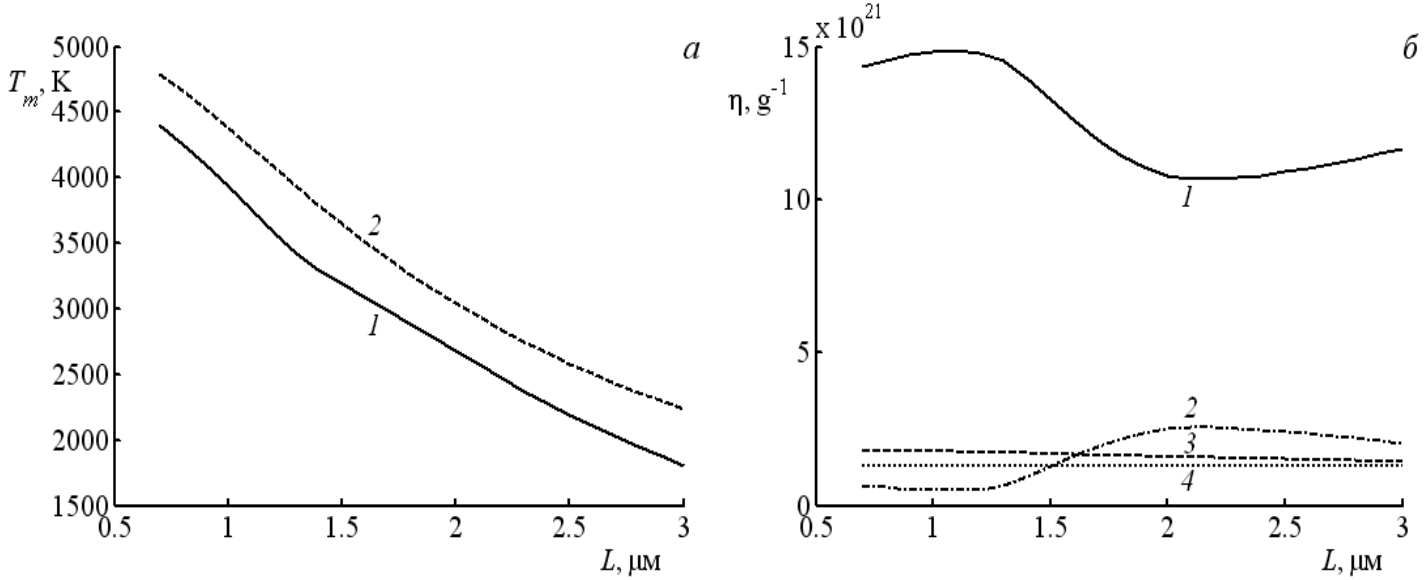
The calculated dependencies of maximum temperature of the particle and products' yields on the energy density of the laser pulse for subbitumenous coal at particle effective radii 1, 3, and 5 μm.

Results (lignite)



The calculated kinetic curves for temperature of the particle and products' concentrations of – CH_2 -CH_2 - (*б*), ethylene (*в*), atomic hydrogen H (*г*), cyclohexadiene fragments in the carbon chain –(C_6H_6)- (*д*), and carbonized matter (*е*) at energy density values 0.7 (*1*), 1.0 (*2*), 1.5 (*3*), and 2.0 J/cm^2 (*4*).

Results (lignite)



The calculated dependencies of maximum temperature (a) taking into account chemical reactions (1) and without them (2) as well as the yields (б) of hydrogen (1), methane (2), carbon monoxide (3), and carbon dioxide (4) on the effective radius of the coal particle.

Conclusion

The model of coal particles' pulsed pyrolysis was suggested that develops the quasipolymeric concept of the coal organic mass. The kinetics of the reactions was modeled and the dependencies of the main products' yields on the energy density of the laser pulse were calculated in the case of subbitumenous coal. The main pyrolysis products are molecular hydrogen and water. The endothermic reactions of the organic mass of coal decomposition lead to the sublinear dependence of the maximum temperature of the particle on the energy density.

Acknowledgments

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Thank you for attention!