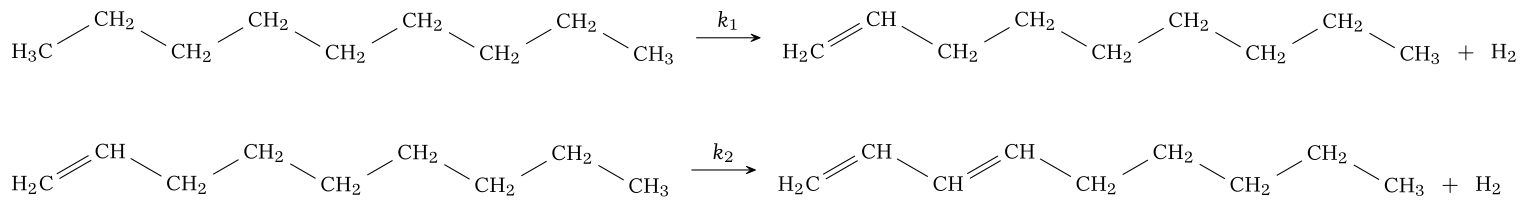
**ЛАБОРАТОРНАЯ РАБОТА № 6**

**Идентификация кинетических параметров при математическом моделировании химических превращений**

**Пример**

Необходимо определить кинетические параметры изменения концентрации каждого компонента в течение 1 часа с шагом 0.1. Концентрация [C9H20 ] в начальный момент времени 1 моль/л, концентрации остальных компонентов равны нулю. Построить зависимость C (t) для каждого компонента.

Схема химических превращений:



Выражения для скоростей химических реакций по закону действующих масс:

Система дифференциальных уравнений для описания изменения концентрации каждого компонента по времени:

Стехиометрическая матрица:

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Реакция |  |  |  |  |
|  |  |  |  |  |
|  |  |  |  |  |

Концентрация компонентов, моль/л:

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Время, ч | C9H20 | C9H18 | C9H16 | H2 |
| 0.1 | 0.8353 | 0.1563 | 0.0084 | 0.1732 |
| 0.2 | 0.6977 | 0.2715 | 0.0308 | 0.3331 |
| 0.3 | 0.5827 | 0.3540 | 0.0633 | 0.4805 |
| 0.4 | 0.4868 | 0.4104 | 0.1028 | 0.6161 |
| 0.5 | 0.4066 | 0.4463 | 0.1471 | 0.7405 |
| 0.6 | 0.3396 | 0.4662 | 0.1942 | 0.8546 |
| 0.7 | 0.2837 | 0.4736 | 0.2427 | 0.9591 |
| 0.8 | 0.2369 | 0.4716 | 0.2915 | 1.0545 |
| 0.9 | 0.1979 | 0.4625 | 0.3396 | 1.1417 |
| 1.0 | 0.1653 | 0.4481 | 0.3866 | 1.2213 |

**Задание**

1. Составьте кинетическую модель в соответствии с представленной схемой превращений.
2. Решите полученную систему дифференциальных уравнений на заданном интервале по времени при заданных начальных концентрациях компонентов, участвующих в химических превращениях, при помощи функции scipy.integrate.solve\_ivp().
3. Определите кинетические параметры химических превращений, используя метод Нелдера-Мида и генетический алгоритм на основе данных по наблюдаемым концентрациям химических веществ, участвующих в реакциях, при различном времени процесса.
4. Постройте зависимости изменения концентраций химических веществ от времени протекания реакций по исходным данным и результатам расчета.

**Вариант 1**

Схема превращений:

Начальные концентрации:

|  |  |  |  |
| --- | --- | --- | --- |
| C10H22 | C10H20 | C10H18 | H2 |
| 1.0 | 0.0 | 0.0 | 0.0 |

Время процесса 1.0 сек.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Время, сек. | C10H22 | C10H20 | C10H18 | H2 |
| 0.0 | 1.000000 | 0.000000 | 0.000000 | 0.000000 |
| 0.1 | 0.882497 | 0.112549 | 0.004954 | 0.122458 |
| 0.2 | 0.778800 | 0.202702 | 0.018498 | 0.239698 |
| 0.3 | 0.687290 | 0.273834 | 0.038876 | 0.351587 |
| 0.4 | 0.606523 | 0.328894 | 0.064583 | 0.458060 |
| 0.5 | 0.535250 | 0.370369 | 0.094381 | 0.559131 |
| 0.6 | 0.472363 | 0.400412 | 0.127225 | 0.654862 |
| 0.7 | 0.416866 | 0.420927 | 0.162207 | 0.745340 |
| 0.8 | 0.367882 | 0.433546 | 0.198571 | 0.830689 |
| 0.9 | 0.324655 | 0.439622 | 0.235723 | 0.911068 |
| 1.0 | 0.286508 | 0.440335 | 0.273157 | 0.986649 |

**Вариант 2**

Схема превращений:

Начальные концентрации:

|  |  |  |  |
| --- | --- | --- | --- |
| C11H24 | C11H22 | C11H20 | H2 |
| 0.8 | 0.1 | 0.1 | 0.0 |

Время процесса 1.0 сек.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Время, сек. | C11H24 | C11H22 | C11H20 | H2 |
| 0.0 | 0.800000 | 0.100000 | 0.100000 | 0.000000 |
| 0.1 | 0.720260 | 0.172199 | 0.107542 | 0.087282 |
| 0.2 | 0.648467 | 0.232803 | 0.118729 | 0.170262 |
| 0.3 | 0.583815 | 0.283238 | 0.132947 | 0.249132 |
| 0.4 | 0.525593 | 0.324735 | 0.149672 | 0.324079 |
| 0.5 | 0.473189 | 0.358338 | 0.168473 | 0.395285 |
| 0.6 | 0.426033 | 0.385012 | 0.188955 | 0.462922 |
| 0.7 | 0.383595 | 0.405651 | 0.210754 | 0.527158 |
| 0.8 | 0.345388 | 0.421070 | 0.233541 | 0.588153 |
| 0.9 | 0.310968 | 0.432005 | 0.257027 | 0.646059 |
| 1.0 | 0.279972 | 0.439030 | 0.280998 | 0.701026 |

**Вариант 3**

Схема превращений:

Начальные концентрации:

|  |  |  |  |
| --- | --- | --- | --- |
| C12H26 | C12H24 | C12H22 | H2 |
| 1.0 | 0.0 | 0.0 | 0.0 |

Время процесса 1.5 сек.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Время, сек. | C12H26 | C12H24 | C12H22 | H2 |
| 0.00 | 1.000000 | 0.000000 | 0.000000 | 0.000000 |
| 0.15 | 0.804527 | 0.180754 | 0.014719 | 0.210193 |
| 0.30 | 0.647262 | 0.300534 | 0.052204 | 0.404941 |
| 0.45 | 0.520733 | 0.374912 | 0.104355 | 0.583622 |
| 0.60 | 0.418956 | 0.415813 | 0.165231 | 0.746276 |
| 0.75 | 0.337032 | 0.432629 | 0.230339 | 0.893307 |
| 0.90 | 0.271153 | 0.432167 | 0.296680 | 1.025527 |
| 1.05 | 0.218183 | 0.419775 | 0.362042 | 1.143859 |
| 1.20 | 0.175526 | 0.399679 | 0.424795 | 1.249269 |
| 1.35 | 0.141217 | 0.374700 | 0.484083 | 1.342866 |
| 1.50 | 0.113622 | 0.347041 | 0.539336 | 1.425714 |

**Вариант 4**

Схема превращений:

Начальные концентрации:

|  |  |  |  |
| --- | --- | --- | --- |
| C13H28 | C13H26 | C13H24 | H2 |
| 1.0 | 0.0 | 0.0 | 0.0 |

Время процесса 2.0 сек.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Время, сек. | C13H28 | C13H26 | C13H24 | H2 |
| 0.0 | 1.000000 | 0.000000 | 0.000000 | 0.000000 |
| 0.2 | 0.637629 | 0.343481 | 0.018890 | 0.381261 |
| 0.4 | 0.406558 | 0.529700 | 0.063742 | 0.657184 |
| 0.6 | 0.259169 | 0.618828 | 0.122003 | 0.862834 |
| 0.8 | 0.165332 | 0.648634 | 0.186034 | 1.020702 |
| 1.0 | 0.105361 | 0.643538 | 0.251101 | 1.145740 |
| 1.2 | 0.067244 | 0.618173 | 0.314583 | 1.247338 |
| 1.4 | 0.042878 | 0.582219 | 0.374904 | 1.332026 |
| 1.6 | 0.027350 | 0.541318 | 0.431333 | 1.403983 |
| 1.8 | 0.017465 | 0.498969 | 0.483566 | 1.466101 |
| 2.0 | 0.011137 | 0.457303 | 0.531560 | 1.520423 |

**Вариант 5**

Схема превращений:

Начальные концентрации:

|  |  |  |  |
| --- | --- | --- | --- |
| C9H16 | H2 | C9H18 | C9H20 |
| 1.0 | 1.0 | 0.0 | 0.0 |

Время процесса 1.0 сек.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Время, сек. | C9H16 | H2 | C9H18 | C9H20 |
| 0.0 | 1.000000 | 1.000000 | 0.000000 | 0.000000 |
| 0.1 | 0.757713 | 0.723147 | 0.207721 | 0.034566 |
| 0.2 | 0.619292 | 0.529340 | 0.290756 | 0.089952 |
| 0.3 | 0.533877 | 0.393634 | 0.325880 | 0.140243 |
| 0.4 | 0.477364 | 0.296735 | 0.342007 | 0.180629 |
| 0.5 | 0.438801 | 0.226331 | 0.348730 | 0.212469 |
| 0.6 | 0.412341 | 0.174581 | 0.349898 | 0.237761 |
| 0.7 | 0.392521 | 0.135459 | 0.350417 | 0.257062 |
| 0.8 | 0.377492 | 0.105570 | 0.350587 | 0.271921 |
| 0.9 | 0.366246 | 0.082733 | 0.350240 | 0.283513 |
| 1.0 | 0.357668 | 0.065073 | 0.349736 | 0.292595 |

**Вариант 6**

Схема превращений:

Начальные концентрации:

|  |  |  |  |
| --- | --- | --- | --- |
| C10H18 | H2 | C10H20 | C10H22 |
| 1.0 | 1.0 | 0.0 | 0.0 |

Время процесса 1.5 сек.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Время, сек. | C10H18 | H2 | C10H20 | C10H22 |
| 0.00 | 1.000000 | 1.000000 | 0.000000 | 0.000000 |
| 0.15 | 0.730661 | 0.695581 | 0.234258 | 0.035081 |
| 0.30 | 0.585666 | 0.496531 | 0.325199 | 0.089135 |
| 0.45 | 0.499750 | 0.362552 | 0.363052 | 0.137198 |
| 0.60 | 0.444211 | 0.269242 | 0.380820 | 0.174969 |
| 0.75 | 0.407159 | 0.202813 | 0.388494 | 0.204347 |
| 0.90 | 0.381326 | 0.154374 | 0.391722 | 0.226952 |
| 1.05 | 0.362391 | 0.118200 | 0.393419 | 0.244190 |
| 1.20 | 0.348597 | 0.091133 | 0.393940 | 0.257464 |
| 1.35 | 0.338337 | 0.070618 | 0.393943 | 0.267720 |
| 1.50 | 0.330515 | 0.054838 | 0.393808 | 0.275677 |

**Вариант 7**

Схема превращений:

Начальные концентрации:

|  |  |  |  |
| --- | --- | --- | --- |
| C11H20 | H2 | C11H22 | C11H24 |
| 1.0 | 1.0 | 0.0 | 0.0 |

Время процесса 2.0 сек.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Время, сек. | C11H20 | H2 | C11H22 | C11H24 |
| 0.0 | 1.000000 | 1.000000 | 0.000000 | 0.000000 |
| 0.2 | 0.707130 | 0.679345 | 0.265086 | 0.027785 |
| 0.4 | 0.555274 | 0.484477 | 0.373928 | 0.070797 |
| 0.6 | 0.467018 | 0.357034 | 0.422998 | 0.109984 |
| 0.8 | 0.409909 | 0.268514 | 0.448696 | 0.141395 |
| 1.0 | 0.371596 | 0.205261 | 0.462068 | 0.166336 |
| 1.2 | 0.344525 | 0.158612 | 0.469563 | 0.185912 |
| 1.4 | 0.324783 | 0.123517 | 0.473951 | 0.201266 |
| 1.6 | 0.310291 | 0.096935 | 0.476354 | 0.213355 |
| 1.8 | 0.299320 | 0.076423 | 0.477782 | 0.222898 |
| 2.0 | 0.290881 | 0.060434 | 0.478672 | 0.230447 |

**Вариант 8**

Схема превращений:

Начальные концентрации:

|  |  |  |  |
| --- | --- | --- | --- |
| C12H22 | H2 | C12H24 | C12H26 |
| 1.0 | 1.0 | 0.0 | 0.0 |

Время процесса 5.0 сек.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Время, сек. | C12H22 | H2 | C12H24 | C12H26 |
| 0.0 | 1.000000 | 1.000000 | 0.000000 | 0.000000 |
| 0.5 | 0.665873 | 0.654674 | 0.322928 | 0.011199 |
| 1.0 | 0.502873 | 0.473974 | 0.468228 | 0.028899 |
| 1.5 | 0.408112 | 0.362414 | 0.546190 | 0.045698 |
| 2.0 | 0.346932 | 0.286602 | 0.592738 | 0.060330 |
| 2.5 | 0.304690 | 0.231873 | 0.622494 | 0.072816 |
| 3.0 | 0.273961 | 0.190562 | 0.642640 | 0.083399 |
| 3.5 | 0.251084 | 0.158682 | 0.656514 | 0.092402 |
| 4.0 | 0.233349 | 0.133286 | 0.666589 | 0.100063 |
| 4.5 | 0.219334 | 0.112734 | 0.674066 | 0.106600 |
| 5.0 | 0.208110 | 0.095911 | 0.679690 | 0.112200 |

**Вариант 9**

Схема превращений:

Начальные концентрации:

|  |  |  |  |
| --- | --- | --- | --- |
| C13H24 | H2 | C13H26 | C13H28 |
| 1.0 | 1.0 | 0.0 | 0.0 |

Время процесса 7.0 сек.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Время, сек. | C13H24 | H2 | C13H26 | C13H28 |
| 0.0 | 1.000000 | 1.000000 | 0.000000 | 0.000000 |
| 0.7 | 0.563595 | 0.544649 | 0.417460 | 0.018946 |
| 1.4 | 0.399424 | 0.356326 | 0.557479 | 0.043098 |
| 2.1 | 0.315918 | 0.253029 | 0.621194 | 0.062889 |
| 2.8 | 0.266229 | 0.187820 | 0.655363 | 0.078409 |
| 3.5 | 0.234218 | 0.143610 | 0.675174 | 0.090608 |
| 4.2 | 0.212004 | 0.111767 | 0.687760 | 0.100236 |
| 4.9 | 0.196215 | 0.088312 | 0.695883 | 0.107903 |
| 5.6 | 0.184474 | 0.070426 | 0.701479 | 0.114047 |
| 6.3 | 0.175556 | 0.056560 | 0.705447 | 0.118997 |
| 7.0 | 0.168693 | 0.045691 | 0.708306 | 0.123001 |

**Вариант 10**

Схема превращений:

Начальные концентрации:

|  |  |  |  |
| --- | --- | --- | --- |
| C6H6 | C9H18 | C6H5(C9H19) | C6H5(C9H19)2 |
| 1.0 | 1.0 | 0.0 | 0.0 |

Время процесса 1.0 сек.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Время, сек. | C6H6 | C9H18 | C6H5(C9H19) | C6H5(C9H19)2 |
| 0.0 | 1.000000 | 1.000000 | 0.000000 | 0.000000 |
| 0.1 | 0.763969 | 0.742402 | 0.214465 | 0.021567 |
| 0.2 | 0.623979 | 0.564771 | 0.316814 | 0.059208 |
| 0.3 | 0.534188 | 0.437880 | 0.369504 | 0.096308 |
| 0.4 | 0.473930 | 0.344740 | 0.396879 | 0.129191 |
| 0.5 | 0.430446 | 0.274286 | 0.413393 | 0.156160 |
| 0.6 | 0.398700 | 0.220262 | 0.422862 | 0.178438 |
| 0.7 | 0.375064 | 0.178274 | 0.428147 | 0.196790 |
| 0.8 | 0.356739 | 0.144984 | 0.431507 | 0.211755 |
| 0.9 | 0.342431 | 0.118421 | 0.433558 | 0.224010 |
| 1.0 | 0.331157 | 0.097082 | 0.434769 | 0.234075 |

**Вариант 11**

Схема превращений:

Начальные концентрации:

|  |  |  |  |
| --- | --- | --- | --- |
| C6H6 | C10H20 | C6H5(C10H20) | C6H5(C10H20)2 |
| 1.0 | 1.0 | 0.0 | 0.0 |

Время процесса 2.0 сек.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Время, сек. | C6H6 | C10H20 | C6H5(C10H20) | C6H5(C10H20)2 |
| 0.0 | 1.000000 | 1.000000 | 0.000000 | 0.000000 |
| 0.2 | 0.644289 | 0.588384 | 0.299805 | 0.055905 |
| 0.4 | 0.493888 | 0.368957 | 0.381180 | 0.124931 |
| 0.6 | 0.416366 | 0.240995 | 0.408263 | 0.175371 |
| 0.8 | 0.372289 | 0.161929 | 0.417350 | 0.210360 |
| 1.0 | 0.344779 | 0.110496 | 0.420939 | 0.234282 |
| 1.2 | 0.327257 | 0.076464 | 0.421950 | 0.250793 |
| 1.4 | 0.315496 | 0.053212 | 0.422219 | 0.262284 |
| 1.6 | 0.307580 | 0.037289 | 0.422129 | 0.270291 |
| 1.8 | 0.302148 | 0.026243 | 0.421948 | 0.275904 |
| 2.0 | 0.298359 | 0.018495 | 0.421777 | 0.279864 |

**Вариант 12**

Схема превращений:

Начальные концентрации:

|  |  |  |  |
| --- | --- | --- | --- |
| C6H6 | C11H22 | C6H5(C11H23) | C6H5(C11H23)2 |
| 1.0 | 1.0 | 0.0 | 0.0 |

Время процесса 3.0 сек.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Время, сек. | C6H6 | C11H22 | C6H5(C11H23) | C6H5(C11H23)2 |
| 0.0 | 1.000000 | 1.000000 | 0.000000 | 0.000000 |
| 0.3 | 0.700735 | 0.664857 | 0.263386 | 0.035878 |
| 0.6 | 0.550138 | 0.461514 | 0.361238 | 0.088624 |
| 0.9 | 0.464910 | 0.330510 | 0.400690 | 0.134400 |
| 1.2 | 0.410900 | 0.241523 | 0.419723 | 0.169377 |
| 1.5 | 0.375600 | 0.179452 | 0.428252 | 0.196148 |
| 1.8 | 0.350991 | 0.134635 | 0.432653 | 0.216356 |
| 2.1 | 0.333537 | 0.101855 | 0.434781 | 0.231682 |
| 2.4 | 0.320982 | 0.077633 | 0.435668 | 0.243350 |
| 2.7 | 0.311626 | 0.059357 | 0.436105 | 0.252269 |
| 3.0 | 0.304640 | 0.045537 | 0.436256 | 0.259104 |

**Вариант 13**

Схема превращений:

Начальные концентрации:

|  |  |  |  |
| --- | --- | --- | --- |
| C10H22 | C10H20 | C10H18 | H2 |
| 1.0 | 0.0 | 0.0 | 0.0 |

Время процесса 3.0 сек.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Время, сек. | C10H22 | C10H20 | C10H18 | H2 |
| 0.0 | 1.000000 | 0.000000 | 0.000000 | 0.000000 |
| 0.3 | 0.798512 | 0.196856 | 0.004631 | 0.206119 |
| 0.6 | 0.637629 | 0.345377 | 0.016993 | 0.379364 |
| 0.9 | 0.509125 | 0.455738 | 0.035136 | 0.526011 |
| 1.2 | 0.406554 | 0.535895 | 0.057551 | 0.650996 |
| 1.5 | 0.324666 | 0.592312 | 0.083021 | 0.758355 |
| 1.8 | 0.259172 | 0.630259 | 0.110569 | 0.851397 |
| 2.1 | 0.206936 | 0.653567 | 0.139498 | 0.932562 |
| 2.4 | 0.165324 | 0.665440 | 0.169236 | 1.003911 |
| 2.7 | 0.132049 | 0.668659 | 0.199291 | 1.067242 |
| 3.0 | 0.105444 | 0.665231 | 0.229326 | 1.123882 |

**Вариант 14**

Схема превращений:

Начальные концентрации:

|  |  |  |  |
| --- | --- | --- | --- |
| C11H24 | C11H22 | C11H20 | H2 |
| 0.8 | 0.1 | 0.1 | 0.0 |

Время процесса 4.0 сек.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Время, сек. | C11H24 | C11H22 | C11H20 | H2 |
| 0.0 | 0.800000 | 0.100000 | 0.100000 | 0.000000 |
| 0.4 | 0.592651 | 0.233285 | 0.174063 | 0.281412 |
| 0.8 | 0.439050 | 0.277354 | 0.283596 | 0.544545 |
| 1.2 | 0.325249 | 0.274252 | 0.400500 | 0.775251 |
| 1.6 | 0.240959 | 0.248230 | 0.510811 | 0.969852 |
| 2.0 | 0.178496 | 0.213638 | 0.607866 | 1.129369 |
| 2.4 | 0.132246 | 0.177654 | 0.690099 | 1.257853 |
| 2.8 | 0.097956 | 0.144498 | 0.757546 | 1.359590 |
| 3.2 | 0.072582 | 0.115378 | 0.812039 | 1.439457 |
| 3.6 | 0.053772 | 0.090998 | 0.855230 | 1.501459 |
| 4.0 | 0.039836 | 0.071047 | 0.889116 | 1.549280 |

**Вариант 15**

Схема превращений:

Начальные концентрации:

|  |  |  |  |
| --- | --- | --- | --- |
| C12H26 | C12H24 | C12H22 | H2 |
| 1.0 | 0.0 | 0.0 | 0.0 |

Время процесса 2.5 сек.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Время, сек. | C12H26 | C12H24 | C12H22 | H2 |
| 0.00 | 1.000000 | 0.000000 | 0.000000 | 0.000000 |
| 0.25 | 0.769126 | 0.179279 | 0.051594 | 0.282468 |
| 0.50 | 0.591555 | 0.246087 | 0.162357 | 0.570802 |
| 0.75 | 0.454978 | 0.254623 | 0.290399 | 0.835421 |
| 1.00 | 0.349938 | 0.235179 | 0.414883 | 1.064945 |
| 1.25 | 0.269144 | 0.204706 | 0.526150 | 1.257006 |
| 1.50 | 0.207007 | 0.171754 | 0.621239 | 1.414232 |
| 1.75 | 0.159211 | 0.140799 | 0.699989 | 1.540778 |
| 2.00 | 0.122460 | 0.113448 | 0.764092 | 1.641632 |
| 2.25 | 0.094184 | 0.090438 | 0.815378 | 1.721194 |
| 2.50 | 0.072444 | 0.071441 | 0.856116 | 1.783672 |

**Вариант 16**

Схема превращений:

Начальные концентрации:

|  |  |  |  |
| --- | --- | --- | --- |
| C13H28 | C13H26 | C13H24 | H2 |
| 1.0 | 0.0 | 0.0 | 0.0 |

Время процесса 3.0 сек.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Время, сек. | C13H28 | C13H26 | C13H24 | H2 |
| 0.0 | 1.000000 | 0.000000 | 0.000000 | 0.000000 |
| 0.3 | 0.509126 | 0.451887 | 0.038987 | 0.529861 |
| 0.6 | 0.259169 | 0.618828 | 0.122003 | 0.862834 |
| 0.9 | 0.132030 | 0.649323 | 0.218647 | 1.086618 |
| 1.2 | 0.067244 | 0.618173 | 0.314583 | 1.247338 |
| 1.5 | 0.034223 | 0.562150 | 0.403627 | 1.369403 |
| 1.8 | 0.017459 | 0.498976 | 0.483564 | 1.466105 |
| 2.1 | 0.008898 | 0.437094 | 0.554008 | 1.545111 |
| 2.4 | 0.004528 | 0.380008 | 0.615464 | 1.610936 |
| 2.7 | 0.002311 | 0.328919 | 0.668770 | 1.666460 |
| 3.0 | 0.001177 | 0.283976 | 0.714846 | 1.713669 |

**Вариант 17**

Схема превращений:

Начальные концентрации:

|  |  |  |  |
| --- | --- | --- | --- |
| C9H16 | H2 | C9H18 | C9H20 |
| 1.0 | 1.0 | 0.0 | 0.0 |

Время процесса 2.0 сек.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Время, сек. | C9H16 | H2 | C9H18 | C9H20 |
| 0.0 | 1.000000 | 1.000000 | 0.000000 | 0.000000 |
| 0.2 | 0.803123 | 0.757841 | 0.196877 | 0.045282 |
| 0.4 | 0.682473 | 0.551843 | 0.317527 | 0.130631 |
| 0.6 | 0.606924 | 0.392091 | 0.393076 | 0.214833 |
| 0.8 | 0.558928 | 0.274084 | 0.441072 | 0.284845 |
| 1.0 | 0.528232 | 0.189702 | 0.471768 | 0.338529 |
| 1.2 | 0.507657 | 0.130401 | 0.492343 | 0.377257 |
| 1.4 | 0.494112 | 0.089270 | 0.505888 | 0.404842 |
| 1.6 | 0.485231 | 0.061124 | 0.514769 | 0.424108 |
| 1.8 | 0.479111 | 0.041679 | 0.520889 | 0.437432 |
| 2.0 | 0.474987 | 0.028393 | 0.525013 | 0.446594 |

**Вариант 18**

Схема превращений:

Начальные концентрации:

|  |  |  |  |
| --- | --- | --- | --- |
| C10H18 | H2 | C10H20 | C10H22 |
| 1.0 | 1.0 | 0.0 | 0.0 |

Время процесса 3.5 сек.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Время, сек. | C10H18 | H2 | C10H20 | C10H22 |
| 0.00 | 1.000000 | 1.000000 | 0.000000 | 0.000000 |
| 0.35 | 0.669667 | 0.617725 | 0.278391 | 0.051942 |
| 0.70 | 0.519913 | 0.400333 | 0.360506 | 0.119581 |
| 1.05 | 0.439948 | 0.268614 | 0.388717 | 0.171334 |
| 1.40 | 0.393167 | 0.184867 | 0.398533 | 0.208300 |
| 1.75 | 0.363478 | 0.129197 | 0.402241 | 0.234281 |
| 2.10 | 0.343967 | 0.091363 | 0.403429 | 0.252604 |
| 2.45 | 0.330791 | 0.065162 | 0.403579 | 0.265629 |
| 2.80 | 0.321604 | 0.046650 | 0.403443 | 0.274954 |
| 3.15 | 0.315225 | 0.033609 | 0.403159 | 0.281616 |
| 3.50 | 0.310685 | 0.024261 | 0.402892 | 0.286423 |

**Вариант 19**

Схема превращений:

Начальные концентрации:

|  |  |  |  |
| --- | --- | --- | --- |
| C11H20 | H2 | C11H22 | C11H24 |
| 1.0 | 1.0 | 0.0 | 0.0 |

Время процесса 2.2 сек.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Время, сек. | C11H20 | H2 | C11H22 | C11H24 |
| 0.00 | 1.000000 | 1.000000 | 0.000000 | 0.000000 |
| 0.22 | 0.661596 | 0.626595 | 0.303402 | 0.035001 |
| 0.44 | 0.505841 | 0.421978 | 0.410297 | 0.083862 |
| 0.66 | 0.420830 | 0.296421 | 0.454761 | 0.124409 |
| 0.88 | 0.369146 | 0.213868 | 0.475576 | 0.155278 |
| 1.10 | 0.335496 | 0.157024 | 0.486033 | 0.178471 |
| 1.32 | 0.312598 | 0.116731 | 0.491536 | 0.195866 |
| 1.54 | 0.296648 | 0.087674 | 0.494378 | 0.208974 |
| 1.76 | 0.285045 | 0.066157 | 0.496067 | 0.218888 |
| 1.98 | 0.276604 | 0.050204 | 0.496995 | 0.226401 |
| 2.20 | 0.270374 | 0.038260 | 0.497512 | 0.232114 |

**Вариант 20**

Схема превращений:

Начальные концентрации:

|  |  |  |  |
| --- | --- | --- | --- |
| C12H22 | H2 | C12H24 | C12H26 |
| 1.0 | 1.0 | 0.0 | 0.0 |

Время процесса 4.0 сек.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Время, сек. | C12H22 | H2 | C12H24 | C12H26 |
| 0.0 | 1.000000 | 1.000000 | 0.000000 | 0.000000 |
| 0.4 | 0.717432 | 0.667358 | 0.232494 | 0.050074 |
| 0.8 | 0.573883 | 0.453738 | 0.305971 | 0.120146 |
| 1.2 | 0.492097 | 0.315587 | 0.331392 | 0.176510 |
| 1.6 | 0.441820 | 0.223638 | 0.339998 | 0.218182 |
| 2.0 | 0.410777 | 0.161311 | 0.339757 | 0.249466 |
| 2.4 | 0.388673 | 0.117277 | 0.339932 | 0.271396 |
| 2.8 | 0.373203 | 0.085929 | 0.339523 | 0.287274 |
| 3.2 | 0.362297 | 0.063390 | 0.338796 | 0.298907 |
| 3.6 | 0.354376 | 0.046883 | 0.338131 | 0.307493 |
| 4.0 | 0.348624 | 0.034786 | 0.337538 | 0.313838 |

**Вариант 21**

Схема превращений:

Начальные концентрации:

|  |  |  |  |
| --- | --- | --- | --- |
| C13H24 | H2 | C13H26 | C13H28 |
| 1.0 | 1.0 | 0.0 | 0.0 |

Время процесса 3.0 сек.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Время, сек. | C13H24 | H2 | C13H26 | C13H28 |
| 0.0 | 1.000000 | 1.000000 | 0.000000 | 0.000000 |
| 0.3 | 0.683586 | 0.650535 | 0.283362 | 0.033051 |
| 0.6 | 0.529644 | 0.448487 | 0.389199 | 0.081157 |
| 0.9 | 0.443570 | 0.320919 | 0.433780 | 0.122651 |
| 1.2 | 0.389621 | 0.234951 | 0.455710 | 0.154670 |
| 1.5 | 0.354340 | 0.175081 | 0.466401 | 0.179259 |
| 1.8 | 0.329748 | 0.131813 | 0.472317 | 0.197935 |
| 2.1 | 0.312437 | 0.100235 | 0.475360 | 0.212203 |
| 2.4 | 0.299854 | 0.076717 | 0.477010 | 0.223136 |
| 2.7 | 0.290481 | 0.058941 | 0.477980 | 0.231540 |
| 3.0 | 0.283471 | 0.045456 | 0.478513 | 0.238016 |

**Вариант 22**

Схема превращений:

Начальные концентрации:

|  |  |  |  |
| --- | --- | --- | --- |
| C6H6 | C9H18 | C6H5(C9H19) | C6H5(C9H19)2 |
| 1.0 | 1.0 | 0.0 | 0.0 |

Время процесса 2.2 сек.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Время, сек. | C6H6 | C9H18 | C6H5(C9H19) | C6H5(C9H19)2 |
| 0.00 | 1.000000 | 1.000000 | 0.000000 | 0.000000 |
| 0.22 | 0.657520 | 0.617898 | 0.302858 | 0.039622 |
| 0.44 | 0.502886 | 0.409475 | 0.403703 | 0.093411 |
| 0.66 | 0.419708 | 0.282886 | 0.443471 | 0.136821 |
| 0.88 | 0.369815 | 0.200738 | 0.461108 | 0.169077 |
| 1.10 | 0.337663 | 0.144882 | 0.469555 | 0.192781 |
| 1.32 | 0.316106 | 0.105897 | 0.473685 | 0.210209 |
| 1.54 | 0.301238 | 0.078151 | 0.475676 | 0.223087 |
| 1.76 | 0.290573 | 0.057922 | 0.476775 | 0.232652 |
| 1.98 | 0.282951 | 0.043194 | 0.477292 | 0.239757 |
| 2.20 | 0.277398 | 0.032336 | 0.477539 | 0.245063 |

**Вариант 23**

Схема превращений:

Начальные концентрации:

|  |  |  |  |
| --- | --- | --- | --- |
| C6H6 | C10H20 | C6H5(C10H20) | C6H5(C10H20)2 |
| 1.0 | 1.0 | 0.0 | 0.0 |

Время процесса 1.5 сек.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Время, сек. | C6H6 | C10H20 | C6H5(C10H20) | C6H5(C10H20)2 |
| 0.00 | 1.000000 | 1.000000 | 0.000000 | 0.000000 |
| 0.15 | 0.734116 | 0.703946 | 0.235714 | 0.030170 |
| 0.30 | 0.588501 | 0.510376 | 0.333374 | 0.078125 |
| 0.45 | 0.501080 | 0.378848 | 0.376688 | 0.122232 |
| 0.60 | 0.443979 | 0.286058 | 0.398100 | 0.157921 |
| 0.75 | 0.404962 | 0.218883 | 0.408960 | 0.186078 |
| 0.90 | 0.377622 | 0.169341 | 0.414096 | 0.208281 |
| 1.05 | 0.357377 | 0.131807 | 0.417054 | 0.225570 |
| 1.20 | 0.342363 | 0.103226 | 0.418500 | 0.239137 |
| 1.35 | 0.331123 | 0.081315 | 0.419070 | 0.249808 |
| 1.50 | 0.322459 | 0.064227 | 0.419310 | 0.258232 |