KINTECH LABORATORY

Calculation of equilibrium composition and temperature of n-decane (kerosene surrogate) combustion products

Background

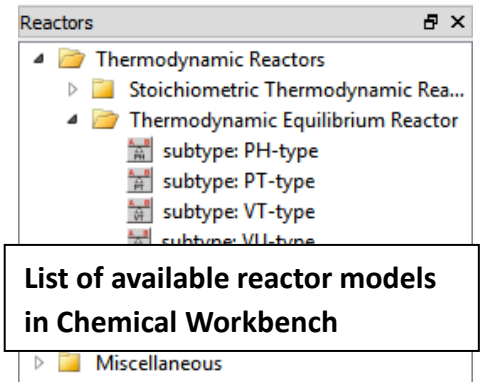
Composition and temperature of the combustion products is an integral part of the analysis of power, energy and transportation systems. It is widely used for efficiency evaluation, thermal analysis, as well as initial guess/conditions for more detailed studies of the systems under consideration.

Problem statement

It is required to calculate equilibrium temperature and composition of the combustion products of aviation kerosene surrogate n-decane C10H22 for a range of mixture equivalence ratio. Initial temperature of kerosene-air is 600K, initial pressure 10 atm. Mixture equivalence ratio is 0.5 – 3.

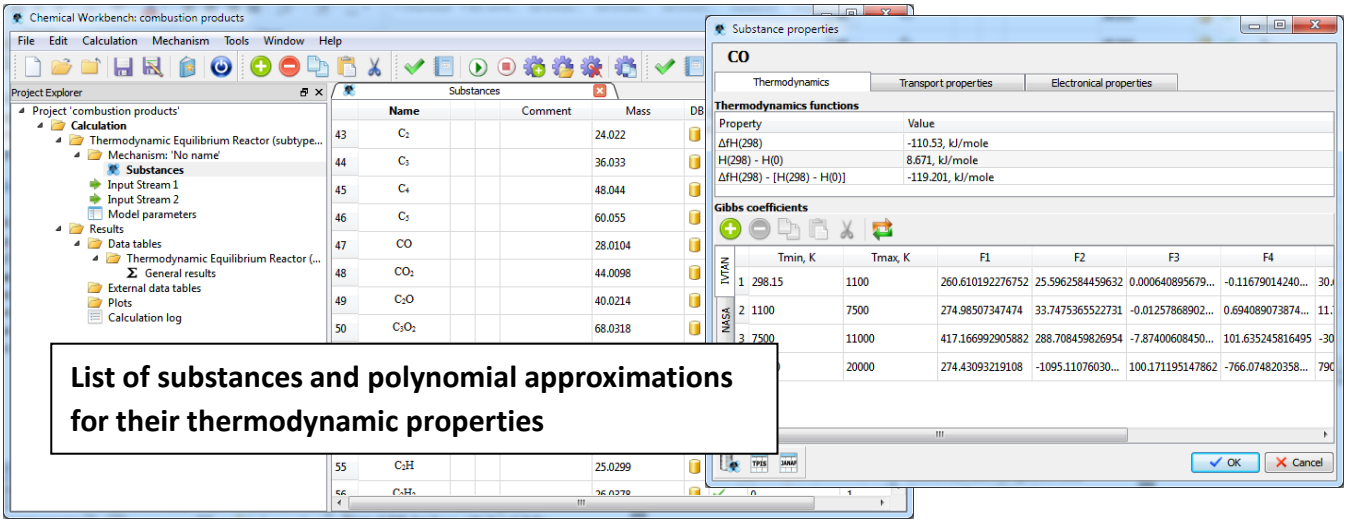
Problem setup in Chemical Workbench

To calculate the equilibrium composition and temperature for n-decane-air combustion, we use the complete **chemical equilibrium model TER_PH (combustion at adiabatic conditions and constant pressure)**, available in Chemical Workbench. This model requires information only about list of all possible products, their thermodynamic properties (specific heat, enthalpy of formation, standard state entropy) and initial conditions. No guess about chemical reaction equations in the system is required



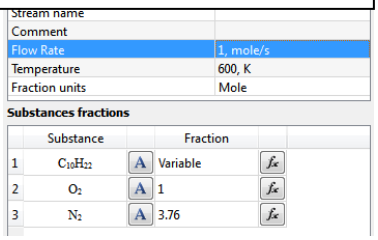
List of available reactor models in Chemical Workbench

The **list of possible combustion products (mechanism)** is generated automatically by query to KintechDB database, which is tightly integrated with Chemical Workbench and provide reference thermodynamic properties data for more than 4100 substances. For n-decane combustion the query to database generates the list of 423 possible substances, composed of elements C, H, O, N , which constitute initial mixture: n-decane ($C_{10}H_{22}$) and air (0.2 O_2 + 0.78 N_2). Their thermodynamic properties are also loaded from database.



List of substances and polynomial approximations for their thermodynamic properties

Initial mixture composition

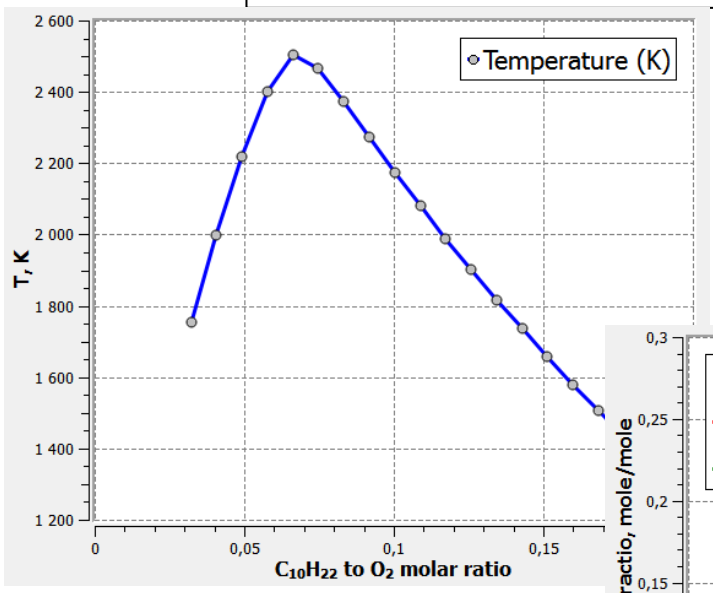


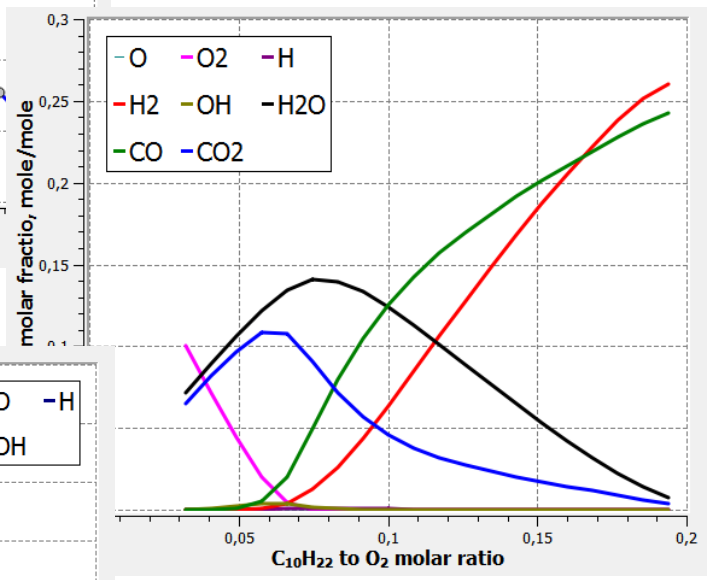
The initial mixture is set in the same input stream of the reactor with composition x$C_{10}H_{22}$ + O_2 + 3.76N_2 (in moles), where x = 0.0322 – 0.194 (φ = 0.5 – 3). **Initial temperature** 600K, **reactor pressure** 10 atm.

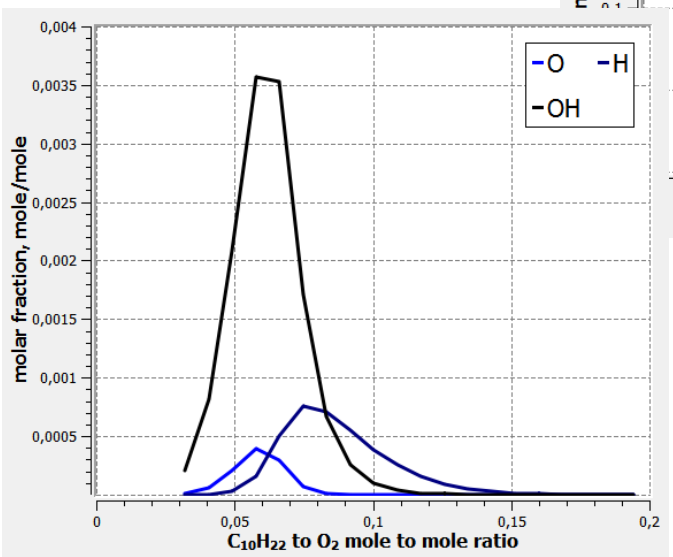
Results

As it would be expected, the maximum temperature of n-decane combustion is achieved at near-stoichiometric conditions. The maximum value (among) of temperature is 2502 K. At fuel-rich conditions the concentration of Co and H_2 increases, while other combustion products are absent due to lack of oxygen. The radicals concentration is low, concentration of H and O is below 0.001 molar fraction, for OH it is of order of several 0.001.

Equilibrium temperature and composition of n-decane/air combustion products: ϕ = 0.5 – 3, T_0 = 600K, P = 10 atm







Next steps

1. Keep only $C_{10}H_{22}$, O_2, N_2, CO, CO_2, H_2, N_2 in the species list and see how the combustion temperature will increase due to lack of dissociation of combustion products
2. Put fuel $C_{10}H_{22}$ with temperature 300K as a separate input stream of TER_PH of reactor model. Allow reactor model automatically account for different temperatures of separate streams. Thus tedious calculation of initial mixture temperature is omitted.