Mathematical formulation of the model

Nomenclature		*watf*	water consumption factor
Set		*f*	technology utilization rate
$t \in T$	time	**Variables**	
$i \in I$	technology	*r*	raw material consumption amount
Parameters		*e*	cumulative installed capacity
disc	discount rate	*c*	installed capacity
cr	raw material cost	*d*	demand
ci	Investment cost	**Decision variables**	
fom	fixed o&m cost	NCAP	newly installed capacity
vom	variable o&m cost	ACT	activity of a technology
τ	technology lifetime		
η	conversion efficiency		
emif	emission factor		

One criteria of our model analysis are the accumulative total cost of the liquid fuel supply system for China's transportation sector from 2020 to 2060. The mathematical expression of total cost is defined by Eq (1)

$$tatalCost = materialCost + investmentCost + OMCost \tag{1}$$

Total cost in our model consists of three parts, which includes:

1) Total raw material cost is defined by Eq (2)

$$marterialCost = \sum_{i \in I} \sum_{t \in T} disc_t \cdot cr_i^t \cdot r_i^t \tag{2}$$

2) Total investment cost, which refers to the cost of building production capacities (i.e., plants) of different technologies and is defined by Eq (3)

$$investmentCost = \sum_{i \in I} \sum_{t \in T} disc_t \cdot ci_i^t \cdot NCAP_i^t \tag{3}$$

3) Total operation and maintenance cost, which donates the cost to maintain the well function of the plant. All costs are occurring in the future, so they are all discounted into the present value of the base year. The mathematical expression is defined by Eq (4)

$$OMCost = \sum_{i \in I} \sum_{t \in T} \sum_{c \in C} disc_t \cdot \left(fom_i^t e_i^t + vom_i^t \cdot ACT_i^t\right) \tag{4}$$

Where *t* is time period (year), $disc_t$ denote the discount rate at time *t*, *i* is technology, cr_i^t is the price of raw material used for technology *i* at time *t*, while r_i^t is the raw material consumption amount of technology *i* at time *t*. ci_i^t is the capital investment for technology *i* at time *t*, while $ncap_i^t$ is newly installed production capacity of technology *i* at time *t*. Similarly, fom_i^t and vom_i^t denote fixed and variable operation and maintenance cost of technology *i* at time *t*. e_i^t is the cumulative installed capacity of technology *i* at time *t*. act_i^t denotes the activity of technology *i* at time *t*.

Since our work is trying to find the way of achieving the carbon-neutral of the liquid fuel supply system for China's transportation sector. So other environmental outcomes or criteria including CO_2 emissions and water consumption are also included. Detailed mathematical expressions in Eq. (5) and Eq. (6).

Outcome 2:

$$CO2 = \sum_{t \in T} \sum_{i \in I} \sum_{c \in C} emif_i \cdot ACT_i^t \tag{5}$$

Outcome 3:

$$Water = \sum_{t \in T} \sum_{i \in I} \sum_{c \in C} watf_i \cdot ACT_i^t \tag{6}$$

Where Eq. (2) denotes CO_2 emission and Eq. (3) represents the water consumption amount. $emif_i$ and $watf_i$ are the emission factor and water consumption factor of technology *i* for at time *t*.

These objects also satisfying with a series of relations and constraints.

Let $r_{i,c}^t$ represent the quantity of the raw material used for producing product *c* at time *t*, is defined by Eq. (7)

$$r_i^t = \frac{ACT_i^t}{\eta_i}, i \in I, t \in T \tag{7}$$

Where $\eta_{i,c}$ is the conversion efficiency of technology *i* for producing product *c*.

c_i^t is the installed capacity of technology *i* at time *t* which is defined by Eq. (8)

$$c_i^t = \begin{matrix} \sum\limits_{t \in [t-\tau_i, T]} NCAP_i^t, t \geq \tau_i \\ \sum\limits_{t \in T} NCAP_i^t + \frac{\tau_i - t}{\tau_i} c_i^0, t \leq \tau_i \end{matrix}, i \in I \tag{8}$$

Where τ_i is the lifetime of technology *i*, c_i^0 is the initial installed capacity.

e_i^t is the cumulative installed capacity of technology *i* at time *t*, which is defined by Eq. (9)

$$e_i^t = e_i^0 + \sum_t^T c_i^t, \{i \in I, \ t \in T\} \tag{9}$$

Where e_i^0 is the initial installed capacity of technology *i*

Additionally, the demand of each type of liquid fuel must be satisfied and can be denoted in Eq. (10)

$$d^t \leq \sum_{i \in I} ACT_i^t, i \in I, t \in T \tag{10}$$

Where d_c^t stands for the demand of the demand at time *t*.

Besides output of the products of the fuel should not exceed the production capacity and is defined by Eq. (11)

$$\sum_{c \in C} ACT_i^t \leq f_i^t c_i^t, i \in I, c \in C, t \in T \tag{11}$$

Where f_i^t is the production capacity utilization rate.