| Nomenclature | | | |
|------------------------|---|--------|--------------------------|
| Set | Meaning | | Numbers in set |
| $y \in Y$ | Year | | 30 |
| $y^v \in Y$ | Year vintage | | 30 |
| $c \in C$ | Commodity | | 8 |
| $t \in T$ | Technology | | 4 |
| $e \in E$ | Emission | | 1 |
| Parameters | Meaning | Unit | Non-zero value range |
| $disc_y$ | Discount | | 0.06 |
| $\omega_{y^{V}}$ | Duration of multi-year period | У | 5-30 |
| $cr_{c,y}$ | Extraction cost for resources | CNY/t | 400-16685 |
| $ci_{t,y}$ | Investment cost | CNY/t | 2578-15495 |
| $fom_{t,y^v,y}$ | Fixed o&m cost | CNY/t | 76.3-774.75 |
| $vom_{t,y^v,y}$ | Variable o&m cost | CNY/t | 2701-8491 |
| $\tau_{t,y}^{}v$ | Technology lifetime | Year | 20-20 |
| $\eta_{t,y}v_{,y,c}$ | Consumption amount of input resources commodity | t/t | 0.0004-12.03 |
| $\alpha_{t,y}v_{,y,c}$ | Production amount of output commodity | t/t | 0.0011-1.05 |
| λ_{t,y^v,y^0} | Factors account for remaining capacity | | 1 |
| $emif_{t,y}v_{,y,e}$ | Emission factor | tC02/t | 0.05-4.75 |
| $f_{t,y}v_{,y}$ | Technology utilization rate | | 0.5-1 |
| $d_{c,y}$ | Demand | t | $2.66-4.16(\times 10^8)$ |
| $c_{t,y}$ | Historical data on new capacity | t | $0.01-2.38(\times 10^8)$ |
| .,, | Variables | | |
| $EXT_{c,y}$ | Resources extraction amount | | t |
| $c_{t,y}v_{,y}$ | Installed capacity | | t |
| totaCost | Total cost | | CNY |
| investmentCost | Total investment cost | | CNY |
| materialCost | Total raw material cost | | CNY |
| OMCost | Total operation and maintenanc | CNY | |
| | Decision variables | | |
| $NCAP_{t,y}$ | Newly installed capacity | t | |
| $ACT_{t,y^{v},y}$ | Activity of a technology t | | |
| $EMISS_{e,t,y}$ | Auxiliary variable for aggregate emissions | | t |
| | by technology type | ί | |
| $S_{c,y}$ | Input or output quantity into intertemporal tommodity stock (storage) | | |

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)

$$tatalCost = materialCost + investmentCost + OMCost$$
 (1)

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

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

$$marterialCost = \sum_{c \in C} \sum_{y \in Y} disc_y \cdot cr_{c,y} \cdot EXT_{c,y}$$
 (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)

$$investmentCost = \sum_{t \in T} \sum_{y \in Y} disc_y \cdot ci_{t,y} \cdot NCAP_{t,y}$$
 (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)

$$OMCost = \sum_{t \in T} \sum_{y \in Y} disc_y \cdot \left(fom_{t, y^v, y} \cdot c_{t, y^v, y} + vom_{t, y^v, y} \cdot ACT_{t, y^v, y} \right)$$
(4)

Where y is time period (year), $disc_y$ the cumulative discount factor over period duration of y years, t is technology, $cr_{c,y}$ is the extraction costs for resources commodity c at year y, while $EXT_{c,y}$ is the resources commodity c extraction amount at time y. $ci_{t,y}$ is the capital investment for technology t at year y, while $NCAP_{t,y}$ is newly installed production capacity of technology t at time y. Similarly, $fom_{t,v^{v},v}$ and $vom_{t,v^{v},v}$ denote fixed and variable operation and maintenance cost of technology t in year y of vintage year y^V . $c_{t.v^v.v}$ is the cumulative installed capacity of technology t in year y of vintage year y^V $ACT_{t,y^v,y}$ denotes the activity of technology t in year y of vintage year y^V .

Other environmental outcomes or criteria including CO2 emissions. Detailed mathematical expressions in Eq. (5).

Outcome 2:

$$EMISS_{e,t,y} = \sum_{t \in T} \sum_{y^{\nu} \le y} emif_{t,y^{\nu},y,e} \cdot ACT_{t,y^{\nu},y}$$
 (5)

Where $emif_i$ is the emission factor of technology i for at time t.

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

Let $EXT_{c,y}$ represent the quantity of the resource commodity c used at year y, the $EXT_{c,y}$ is defined by Eq. (6)

$$EXT_{c,y} = \sum_{t} \sum_{y^{v} \le y} \eta_{t,y^{v},y,c} \cdot ACT_{t,y^{v},y}$$
 (6)

Where $\eta_{t,y}v_{,y,c}$ is the input amount of resources commodity c by technology t in year y at vintage year y^V .

Besides, the actual activity of a technology cannot exceed available (maintained) capacity, including the technology capacity factor, which is denoted by Eq. (7)

$$ACT_{t,v}v_{,v} \le f_{t,v}v_{,v} \cdot c_{t,v}v_{,v} \tag{7}$$

 $ACT_{t,y^V,y} \leq f_{t,y^V,y} \cdot c_{t,y^V,y}$ Where $f_{t,y^V,y}$ is the capacity factor of technology t in year y vintage year y^V .

Let $c_{t,y^V,y}$ denote the installed capacity of technology t at year y, then $c_{t,y^V,y}$ satisfied with following constrict and relations:

The first constraint ensures that historical capacity (built prior to the model horizon) is available as installed capacity in the first model period.

$$c_{t,y}v_{,y^0} \leq \lambda_{t,y^v,y^0} \cdot \omega_y v \cdot c_{t,y^0}$$

$$y^{V} < y^{0}$$
 and $|y| - |y^{V}| < \tau_{t, y^{V}}$ (8)

The second constraint ensures that capacity is fully maintained throughout the model period in which it was constructed (no early retirement in the period of construction).

$$c_{t,y^{V},y^{V}} = \lambda_{t,y^{V},y^{0}} \cdot \omega_{y^{V}} \cdot NCAP_{t,y^{V},y-1}$$

$$\tag{9}$$

The third constraint implements the dynamics of capacity maintenance throughout the model horizon. Installed capacity can be maintained over time until decommissioning, which is irreversible.

$$c_{t,y^{V},y} = \lambda_{t,y^{v},y} \cdot NACP_{t,y^{V},y-1}$$

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$$y > y^{V} \text{ and } y^{V} > \text{ and } |y| - |y^{V}| < \tau_{t,y^{V}}$$
 (10)

Let $d_{c,y}$ to be the fixed demand, then the demand of different commodity c at year y must be satisfied which can be denote in Eq. (11)

$$\sum_{t} \sum_{y^{v} \le y} \alpha_{t,y^{v},y,c} \cdot ACT_{t,y^{v},y} - \sum_{t} \sum_{y^{v} \le y} \eta_{t,y^{v},y,c} \cdot ACT_{t,y^{v},y} + S_{c,y} = d_{c,y}$$
 (11)

Where $\alpha_{t,y}v_{,y,c}$ and $\eta_{t,y}v_{,y,c}$ are the output commodity production and input commodity consumption amount by technology t for producing commodity c in year y with vintage year y^V .

Dictionary between specs03 and MESSAGE document

| Nomenclature in Specs03 | Nomenclature in MESSAGE Document | Meaning |
|---|----------------------------------|---|
| | Set | Meaning |
| $y \in Y$ | $y \in Y$ | Year |
| $y^v \in Y$ | $y^{v} \in Y$ | Year vintage |
| $c \in C$ | $c \in C$ | Commodity |
| $t \in T$ | $t \in T$ | Technology |
| $e \in E$ | $e \in E$ | Emission |
| Pa | arameters | Meaning |
| $disc_y$ | df_period | Discount |
| $\omega_{\mathcal{y}}v$ | duration_period | Duration of multi-year period |
| $\mathit{cr}_{c,y}$ | resource_cost | Extraction cost for resources |
| $ci_{t,y}$ | inv_cost | Investment cost |
| $fom_{t, \mathcal{Y}^{\mathcal{v}}, \mathcal{Y}}$ | fix_cost | Fixed o&m cost |
| $vom_{t, \mathcal{Y}^{v}, \mathcal{Y}}$ | var_cost | Variable o&m cost |
| $	au_{t,\mathcal{Y}}v$ | $technologica_lifetime$ | Technology lifetime |
| $\eta_{t,y}v_{,y,c}$ | input | Consumption amount of input resources commodity |
| $lpha_{t,y}v_{,y,c}$ | output | Production amount of output commodity |
| $\lambda_{t, \mathcal{Y}^{oldsymbol{v}}, \mathcal{Y}^{oldsymbol{0}}}$ o | remain_capacity | Factors account for remaining capacity |
| $emif_{t,y}v_{,y,e}$ | $emission_factor$ | Emission factor |
| $f_{t,y}v_{,y}$ | $capacity_factor$ | Technology utilization rate |
| $d_{c,\mathcal{Y}}$ | $demand_fixed$ | Demand |
| $c_{t,y}$ o | historical_new_capacity | Historical data on new capacity |
| V | /ariables | Meaning |
| $EXT_{c,y}$ | EXT | Resources extraction amount |
| $c_{t,y^{v},y}$ | CAP | Installed capacity |

| totaCost | totaCost | Total cost |
|-------------------|----------------|---|
| investmentCost | investmentCost | Total investment cost |
| materialCost | materialCost | Total raw material cost |
| OMCost | OMCost | Total operation and maintenance cost |
| Decision v | ariables | Meaning |
| $NCAP_{t,y}$ | CAP_NEW | Newly installed capacity |
| $ACT_{t,y^{v},y}$ | ACT | Activity of a technology |
| $EMISS_{e,t,y}$ | EMISS | Auxiliary variable for aggregate emissions by technology type |
| $S_{c,y}$ | STOCK_CHG | Input or output quantity into intertemporal commodity stock (storage) |