Instructions for *IAST Calculator*

Users can launch the **IASTCalculator.m** file to access the interface as shown in Fig.1. Based on Eq. (1), the expressions for the spreading pressure of each component in the mixtures can be derived using the isotherms of the pure component. Within the framework of IAST, there are also certain limitations on thermodynamic equilibrium relationship, demonstrated as Eqs. (2) – (4). Therefore, we can get a system of $N+1$ integral equations, which involves $N+1$ unknowns, including the spreading pressure and the molar fractions in the adsorbed phase for N components. Then the **fsolve** function in MATLAB is implemented to numerically solve the system and determine the molar fractions of each component in the adsorbed phase. Finally, by substituting the results into each equation, other adsorption data can be calculated in the mixtures, including the spreading pressure, the pure component pressure P^0 and total and each component's adsorbed amount.

$$\pi_i^* = \frac{\pi_i A}{RT} = \int_0^{P_i^0} q_i^0 d(\ln P_i^0) = \text{constant}, \quad i = 1,2,\dots,\text{N} \tag{1}$$

$$Py_i = P_i^0 x_i \tag{2}$$

$$\sum_i^N x_i = 1 \tag{3}$$

$$\frac{1}{q_t} = \sum_i^{\text{N}} \frac{x_i}{q_i^0} \tag{4}$$

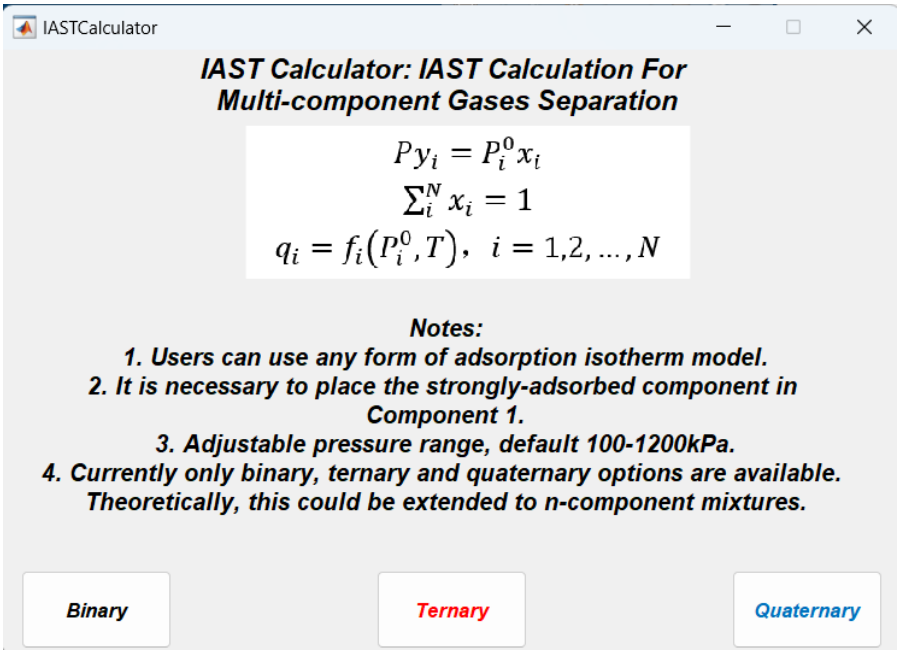

Fig. 1. Start-up interface of *IAST Calculator* software.

Taking "**Quaternary**" as an example, as shown in Fig. 2, we will explain the software usage here. In the "Input" module, the adsorption isotherms and mole fractions of each pure component gas are entered in the "**Users' Defined Isotherm Model**" and "**yi**" columns, respectively. For researchers without coding experience, the isotherm model can be input in any user-defined format, allowing flexibility in choosing the model that best fits the experimental data. There is no need to focus on common or uncommon models. Notably, the gases should be listed in descending order of adsorption strength. In the "**Calculation**" module, once a pressure value is entered in the "**P**" column, clicking the "**RUN**" button will calculate the adsorption amount of each component for the given pressure. The calculated results of molar fractions and adsorbed amounts are shown in the "$\boldsymbol{x_i}$" and "$\boldsymbol{n_i}$" columns, respectively. For a broader pressure range, after entering the model and data, pressing the "**Output Excel files**" button generates an Excel file with adsorption results for pressures between 100-1200 kPa, including the molar fraction (x_i) and the adsorbed amount (n_i). This range is typical for gas separation using PSA, but users can adjust the pressure range in the m-file as needed.

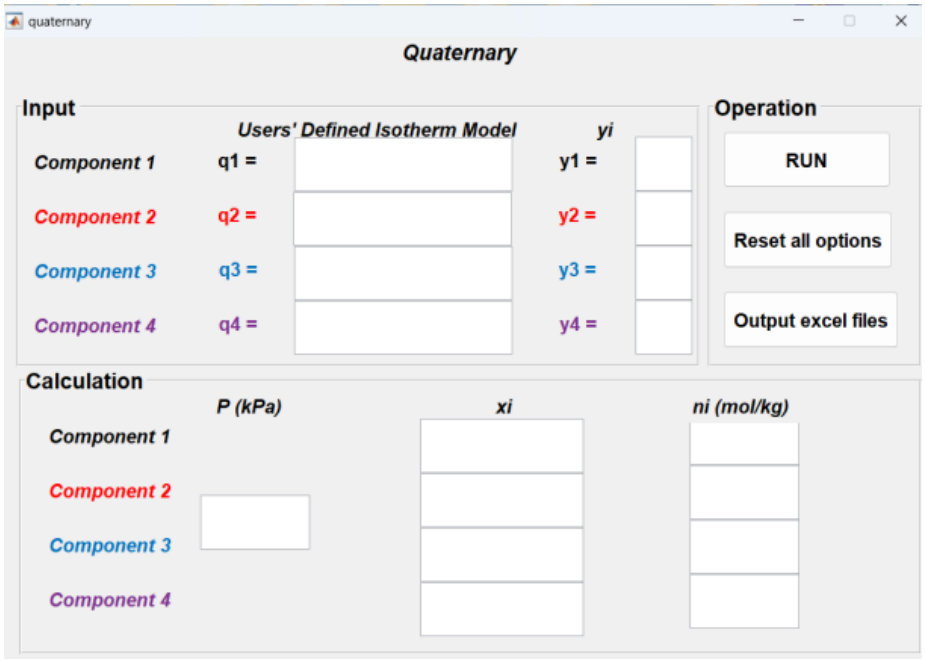

Fig. 2. the interface of IAST calculation program.