APPENDIX

A. Derivation of Hydrogen Component Transfer Equation

Expression of hydrogen mass fraction is shown as (A1). Equation (A2) and (A3) are the continuity equation of gas mixture and hydrogen component respectively.

$$\phi_h = \frac{m}{M} = \frac{\rho_h \omega A}{\rho \omega A} = \frac{\rho_h}{\rho} \tag{A1}$$

$$\frac{\partial \rho}{\partial t} + \nabla(\rho\omega) = 0 \tag{A2}$$

$$\frac{\partial \rho_h}{\partial t} + \nabla(\rho_h \omega) = 0 \tag{A3}$$

By substituting ρ_h in (A3) with (A1), equation (A4) can be derived.

$$\rho\frac{\partial \phi_h}{\partial t} + \phi_h \frac{\partial \rho}{\partial t} + \rho\omega\nabla\phi_h + \phi_h \nabla\rho\omega = 0 \tag{A4}$$

Combining (A2) and (A4), the hydrogen component transfer equation can be derived.

$$\frac{\partial \phi_h}{\partial t} + \omega\frac{\partial \phi_h}{\partial x} = 0 \tag{A5}$$

B. Difference form of Hydrogen Component Transfer Equation

(A3) can also be expressed as

$$\frac{\partial \rho\phi_h}{\partial t} + \nabla(\rho\phi_h\omega) = 0 \tag{A6}$$

To reformulate (A6) in the form of *m*, replace $\rho\phi_h$ with the corresponding expression involving $\rho\phi_h\omega$.

$$\frac{\partial \rho\phi_h\omega}{\partial t} = \omega\frac{\partial \rho\phi_h}{\partial t} + \phi_h\frac{\partial \rho\omega}{\partial t} \tag{A7}$$

Combining (A6) and (A7), it can be referred that

$$\frac{1}{\omega}\left(\frac{\partial \rho\phi_h\omega}{\partial t} - \phi_h\frac{\partial \rho\omega}{\partial t}\right) + \frac{\partial \rho\phi_h\omega}{\partial x} = 0 \tag{A8}$$

m can be expressed as $m = \rho\phi_h\omega A$, ϕ_h can be replaced in the form of *m* and *M*, so

$$\frac{\partial m}{\partial t} + \omega\frac{\partial m}{\partial x} - \frac{m}{M}\frac{\partial M}{\partial t} = 0 \tag{A9}$$

C. Derivation of Differential Stability Conditions

When determining the size of the discretization cells, two criteria should be considered: firstly, satisfying the CFL condition (A10). The CFL condition restricts the time step size based on the grid spacing and the maximum wave speed, and violating it can lead to numerical instability. For the explicit upwind differencing scheme applied to the one-dimensional linear convection equation, the Courant number *C* is typically set to 1.

$$\gamma_{cfl} = \frac{\omega\Delta t}{\Delta x} \le C \tag{A10}$$

Secondly, satisfying stability conditions of the component transport equation, which is a convection equation. The spatial grid must be sufficiently dense to avoid severe numerical oscillations, known as the Gibbs phenomenon, and prevent noticeable overshooting and undershooting.

For the convenience of deriving stability conditions, transform the original form of the hydrogen component transfer equation (A5). First, use the first-order upwind scheme for discretization:

$$\begin{aligned}&\frac{1}{2\Delta t}\left(\phi_{Fl,t} + \phi_{El,t} - \phi_{Fl,t-1} - \phi_{El,t-1}\right)\\&+\frac{1}{2\Delta x}\left(\overline{\omega}_{Fl,t} + \overline{\omega}_{El,t}\right)\left(\phi_{El,t} - \phi_{Fl,t}\right) = 0\end{aligned} \tag{A11}$$

It can be derived that

$$K = \frac{\Delta t}{\Delta x}\left(\overline{\omega}_{Fl,t} + \overline{\omega}_{El,t}\right) \tag{A12}$$

$$(K+1)\phi_{El,t} + (1-K)\phi_{Fl,t} - \phi_{El,t-1} - \phi_{Fl,t-1} = 0 \tag{A13}$$

$$\begin{aligned}&K\left(\phi_{El,t-1} - \phi_{Fl,t-1}\right) + (1-K)\left(\phi_{Fl,t} - \phi_{Fl,t-1}\right)\\&+(K+1)\left(\phi_{El,t} - \phi_{El,t-1}\right) = 0\end{aligned} \tag{A14}$$

$$\left(\phi_{El,t} - \phi_{El,t-1}\right) + \frac{K}{K+1}\left(\phi_{El,t-1} - \phi_{Fl,t-1}\right) = \frac{K-1}{K+1}\left(\phi_{Fl,t} - \phi_{Fl,t-1}\right) \tag{A15}$$

When a sudden change occurs, meeting the condition $K-1>0$ can prevent false numerical oscillations. The detailed derivation process is as follows.

First, in a randomly picked case, the trend of hydrogen mass fraction changes at downstream nodes should be consistent with those upstream nodes. Namely, $\phi_{Fl,t} - \phi_{Fl,t-1}$ should have the same sign as $\phi_{El,t} - \phi_{El,t-1}$.

Then, when the hydrogen blending remains steady for a period, components are uniformly distributed at both the beginning and end of the pipeline, $\phi_{El,t-1} = \phi_{Fl,t-1} = \phi_0$. According to (A15), whether $\phi_{El,t} - \phi_{El,t-1}$ and $\phi_{Fl,t} - \phi_{Fl,t-1}$ have the same sign depends on whether $K > 1$ is satisfied. If the signs of the two mentioned terms are opposite, the trends of upstream and downstream changes are opposite, that is, numerical oscillation occurs.

Therefore, when discretizing the grid, the spatial step size Δx should satisfy the threshold condition:

$$\frac{\left(\omega_{Fl,t} + \omega_{El,t}\right)}{2}\Delta t \le x \le \Delta t\left(\omega_{Fl,t} + \omega_{El,t}\right) \tag{A16}$$

D. Simplified Form of Bi-level Optimization

The simplified form of objective is:

$$\min\sum_{t\in\mathcal{T}}\left[\begin{aligned}&\sum_{g\in\mathcal{G}^{\mathrm{CFU}}} c_{g,t}^{\mathrm{CFU}} P_{g,t}^{\mathrm{CFU}} - \sum_{g\in\mathcal{G}^{\mathrm{EL}}} c_{g,t}^{\mathrm{EL}} P_{g,t}^{\mathrm{EL}}\\&+\sum_{g\in\mathcal{G}^{\mathrm{WF}}} c_{g,t}^{\mathrm{wcur}}\left(\overline{P}_{g,t}^{\mathrm{WF}} - P_{g,t}^{\mathrm{WF}}\right) + \sum_{g\in\mathcal{G}^{\mathrm{EL}}} c_{g,t}^{\mathrm{shed}}\left(\overline{P}_{g,t}^{\mathrm{EL}} - P_{g,t}^{\mathrm{EL}}\right) + X\end{aligned}\right]$$

(A17)

$$\begin{aligned}X =& \sum_{g\in\mathcal{G}^{\mathrm{CFU}}}\left(c_{g,t}^{\mathrm{GFU}} + \lambda_{g,t}^{\mathrm{GFU}}\right)P_{g,t}^{\mathrm{GFU}} - \sum_{g\in\mathcal{G}^{\mathrm{P2H}}}\left(c_{g,t}^{\mathrm{P2H}} + \lambda_{g,t}^{\mathrm{P2H}}\right)P_{g,t}^{\mathrm{P2H}}\\
=& \sum_{g\in\mathcal{G}^{\mathrm{GFU}}} e_{g,t}^{\mathrm{GFU}} P_{g,t}^{\mathrm{GFU}} / \eta_{g,t}^{\mathrm{GFU}} + P_{g,t}^{\mathrm{GFU}} Q_{g,t}^{\mathrm{GFU}} P_{g,t}^{\mathrm{GFU}} + \overline{P}_{g,t}^{\mathrm{GFU}}\overline{\mu}_{g,t}^{\mathrm{GFU}}\\
&- \sum_{g\in\mathcal{G}^{\mathrm{P2H}}} e_{n,t}^{\mathrm{P2H}} P_{n,t}^{\mathrm{P2H}} \eta_{n,t}^{\mathrm{P2H}} + P_{n,t}^{\mathrm{P2H}} Q_{g,t}^{\mathrm{P2H}} P_{g,t}^{\mathrm{P2H}} + \overline{P}_{g,t}^{\mathrm{P2H}}\overline{\mu}_{g,t}^{\mathrm{P2H}}\\
&+\sum_{r}^{2m+n}\overline{\boldsymbol{\pi}}_{Gr}\left[\overline{\boldsymbol{\Pi}}_G - \boldsymbol{S}_{Gr}^{b}\boldsymbol{b}_G^{0} + \alpha\left(\boldsymbol{S}_{Gr}^{\mathrm{GFU}}\boldsymbol{S}_{Hr,\mathrm{GFU}}^{b} + \boldsymbol{S}_{Gr}^{b}\boldsymbol{S}_{Hr,b}^{b}\right)\boldsymbol{b}_H\right]\\
&-\sum_{r}^{2m+n}\underline{\boldsymbol{\pi}}_{Gr}\left[\underline{\boldsymbol{\Pi}}_G - \boldsymbol{S}_{Gr}^{b}\boldsymbol{b}_G^{0} + \alpha\left(\boldsymbol{S}_{Gr}^{\mathrm{GFU}}\boldsymbol{S}_{Hr,\mathrm{GFU}}^{b} + \boldsymbol{S}_{Gr}^{b}\boldsymbol{S}_{Hr,b}^{b}\right)\boldsymbol{b}_H\right]\\
&+\sum_{r}^{2m}\overline{\boldsymbol{\pi}}_{Hr}\left[\overline{\phi}_{r,t}\left(\boldsymbol{S}_{Gr}^{b}\boldsymbol{b}_G^{0} - \alpha\left(\boldsymbol{S}_{Hr,\mathrm{GFU}}^{b}\boldsymbol{S}_{Gr}^{\mathrm{GFU}} + \boldsymbol{S}_{Gr}^{b}\boldsymbol{S}_{Hr,b}^{b}\right)\boldsymbol{b}_H\right) - \boldsymbol{S}_{Hr}^{b}\boldsymbol{b}_H\right]\\
&+\sum_{r}^{2m}\underline{\boldsymbol{\pi}}_{Hr}\left[\boldsymbol{S}_{Hr}^{b}\boldsymbol{b}_H - \underline{\phi}_{r,t}\left(\boldsymbol{S}_{Gr}^{b}\boldsymbol{b}_G^{0} - \alpha\left(\boldsymbol{S}_{Gr}^{\mathrm{GFU}}\boldsymbol{S}_{Hr,\mathrm{GFU}}^{b} + \boldsymbol{S}_{Gr}^{b}\boldsymbol{S}_{Hr,b}^{b}\right)\boldsymbol{b}_H\right)\right]\end{aligned}$$

(A18)

The constraints are divided into two parts: the upper-level constraints and the equilibrium constraints of the lower level. Detailed forms of the equilibrium constraints are as follows:

$$\begin{aligned}\frac{\partial L_{lower}}{\partial P_{g,t}^{\mathrm{GFU}}} &= -\left(c_{g,t}^{\mathrm{GFU}} + \lambda_{g,t}^{\mathrm{GFU}}\right) + e_{g,t}^{\mathrm{GFU}} / \eta_{g}^{\mathrm{GFU},0} + Q_{g,t}^{\mathrm{GFU}} P_{g,t}^{\mathrm{GFU}} \\ &- \underline{\mu}_{g,t}^{\mathrm{GFU}} + \overline{\mu}_{g,t}^{\mathrm{GFU}} + \sum_{r}^{2m+n}\left(\overline{\pi}_{Gr,t}^{\mathrm{GFU}} - \underline{\pi}_{Gr,t}^{\mathrm{GFU}}\right) S_{Gr,g,t}^{\mathrm{GFU}} / \eta_{g}^{\mathrm{GFU},0} \\ &+ \sum_{r}^{2m}\left(\underline{\pi}_{Hr,t}\underline{\phi}_{r,t} - \overline{\pi}_{Hr,t}\overline{\phi}_{r,t}\right) S_{Gr,g,t}^{\mathrm{GFU}} / \eta_{g}^{\mathrm{GFU},0} = 0\end{aligned} \tag{A19}$$

$$\begin{aligned}\frac{\partial L_{lower}}{\partial P_{g,t}^{\mathrm{P2H}}} &= \left(c_{g,t}^{\mathrm{P2H}} - \lambda_{g,t}^{\mathrm{P2H}}\right) - e_{g,t}^{\mathrm{P2H}}\eta_{g,t}^{\mathrm{P2H}} + Q_{g,t}^{\mathrm{P2H}} P_{g,t}^{\mathrm{P2H}} - \underline{\mu}_{g,t}^{\mathrm{P2H}} + \overline{\mu}_{g,t}^{\mathrm{P2H}} \\ &+ \sum_{r}^{2m+n}\left(\overline{\pi}_{Gr,t} - \underline{\pi}_{Gr,t}\right) S_{Gr}^{\mathrm{P2H}}\eta_{g,t}^{\mathrm{P2H}} + \sum_{r}^{2m}\left(\overline{\pi}_{Hr,t} - \underline{\pi}_{Hr,t}\right) S_{Hr}^{\mathrm{P2H}}\eta_{g,t}^{\mathrm{P2H}} \\ &+ \sum_{r}^{2m+n}\left(\overline{\pi}_{Gr,t} - \underline{\pi}_{Gr,t}\right)\left[-S_{Gr}^{\mathrm{GFU}}\left(\alpha S_{H,\mathrm{GFU}}^{\mathrm{P2H}}\eta_{g,t}^{\mathrm{P2H}}\right) - S_{Gr}^{b}\left(\alpha S_{H,b}^{\mathrm{P2H}}\eta_{g,t}^{\mathrm{P2H}}\right)\right] \\ &+ \sum_{r}^{2m}\left(-\overline{\pi}_{Hr,t}\overline{\phi} + \underline{\pi}_{Hr,t}\underline{\phi}\right)\left[S_{Gr}^{\mathrm{P2H}}\eta_{g,t}^{\mathrm{P2H}} - S_{Gr}^{\mathrm{GFU}}\left(\alpha S_{H,\mathrm{GFU}}^{\mathrm{P2H}}\eta_{g,t}^{\mathrm{P2H}}\right) - S_{Gr}^{b}\left(\alpha S_{H,b}^{\mathrm{P2H}}\eta_{g,t}^{\mathrm{P2H}}\right)\right]\end{aligned} \tag{A20}$$

$$\begin{aligned}0 \le P_{g,t}^{\mathrm{GFU}} \perp \underline{\mu}_{g,t}^{\mathrm{GFU}} \ge 0 \\ 0 \le \overline{P}_{g,t}^{\mathrm{GFU}} - P_{g,t}^{\mathrm{GFU}} \perp \overline{\mu}_{g,t}^{\mathrm{GFU}} \ge 0\end{aligned} \tag{A21}$$

$$\begin{aligned}0 \le P_{g,t}^{\mathrm{P2H}} \perp \underline{\mu}_{g,t}^{\mathrm{P2H}} \ge 0 \\ 0 \le \overline{P}_{g,t}^{\mathrm{P2H}} - P_{g,t}^{\mathrm{P2H}} \perp \overline{\mu}_{g,t}^{\mathrm{P2H}} \ge 0\end{aligned} \tag{A22}$$

$$\begin{aligned}0 \le \mathbf{\Pi}_{G} - \underline{\mathbf{\Pi}}_{G} \perp \underline{\boldsymbol{\pi}}_{G} \ge 0 \\ 0 \le \overline{\mathbf{\Pi}}_{G} - \mathbf{\Pi}_{G} \perp \overline{\boldsymbol{\pi}}_{G} \ge 0\end{aligned} \tag{A23}$$

$$\begin{aligned}0 \le \boldsymbol{S}_{H}^{\mathrm{P2H}}\boldsymbol{M}^{\mathrm{P2H}} + \boldsymbol{S}_{H}^{b}\boldsymbol{b}_{H} - \underline{\phi}\,\Pi_{G}^{M} \perp \underline{\boldsymbol{\pi}}_{H} \ge 0 \\ 0 \le \overline{\phi}\,\Pi_{G}^{M} - \boldsymbol{S}_{H}^{\mathrm{P2H}}\boldsymbol{M}^{\mathrm{P2H}h} - \boldsymbol{S}_{H}^{b}\boldsymbol{b}_{H} \perp \overline{\boldsymbol{\pi}}_{H} \ge 0\end{aligned} \tag{A24}$$

For example, complementary slackness conditions can be reformulated as

$$0 \le P_{g,t}^{\mathrm{GFU}} \le \delta_{g,t}^{\mathrm{GFU,min}} M^{P} \tag{A25}$$

$$0 \le \underline{\mu}_{g,t}^{\mathrm{GFU}} \le \left(1 - \delta_{g,t}^{\mathrm{GFU,min}}\right) M^{D} \tag{A26}$$

$$0 \le P_{g}^{\mathrm{GFU,max}} - P_{g,t}^{\mathrm{GFU}} \le \delta_{g,t}^{\mathrm{GFU,max}} M^{P} \tag{A27}$$

$$0 \le \overline{\mu}_{g,t}^{\mathrm{GFU}} \le \left(1 - \delta_{g,t}^{\mathrm{GFU,max}}\right) M^{D} \tag{A28}$$