Appendix A Estimation of molecular diffusion velocities s_D

To estimate the magnitude of the molecular diffusion velocities s_D, an approximation of $\overline{\rho D_c \nabla c} \approx \overline{\rho} \tilde{D}_c \nabla \tilde{c}$ was applied, with errors coming from two resources. The one is the neglecting the Favre-correlation term of $\widetilde{D_c'' \frac{\partial c''}{\partial x}}$ in the approximation, which may overestimate the molecular diffusion flux. The other one is the overestimation of $\nabla \tilde{c}$ when applying the thin flamelet assumption. Overall, the following analysis only enables us to estimate the order of the negligible molecular diffusion flux to be compared with other terms, but cannot provide an accurate measurement of the molecular diffusion unless we have a full measurement of the progress of reaction c in every single shot.

A.1 Molecular diffusion flux

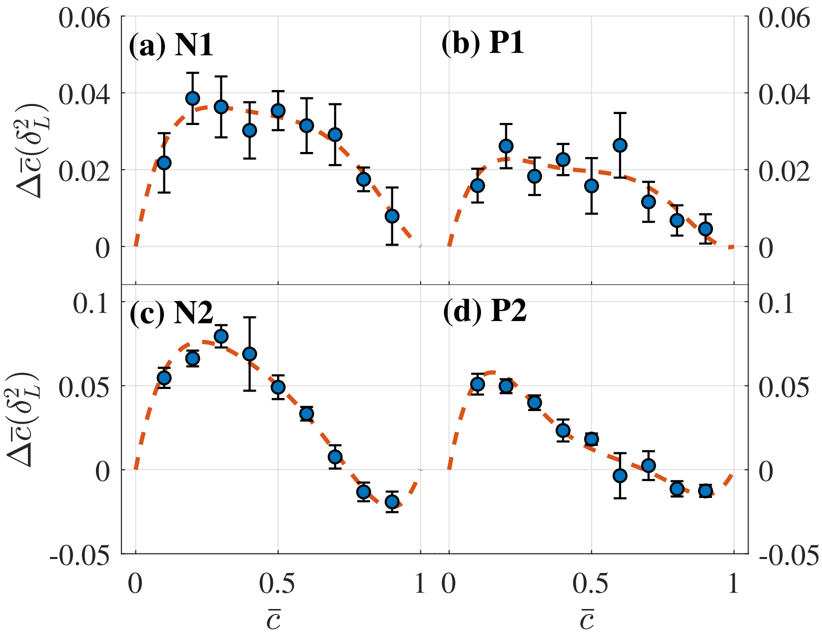

Fig. A2 Laplacian operator of $\overline{c}$ along selected streamlines, normalized by δ_L^2. Blue solid symbol: conditional average of $\Delta\overline{c}$; red dash line: Fitting with Eq. (A16).

The final (and as will be seen, smallest) term to be estimated is the molecular diffusion term $\nabla \cdot \mathbf{T_c^D}$ in Eq. 4 using the bimodal flamelet model by Libby Libby (1989) to consider the effect of temperature on diffusivity. The approximation assumes that the mean diffusion flux is of the order of the diffusion flux of the mean Dunstan et al (2011), to obtain the order of magnitude of the term, and the molecular diffusion coefficient is equal to the thermal diffusivity as Lewis number equal to one, scaled with temperature via Sutherland's law ($T^{3/2}$). The molecular diffusion flux T_c^D can be modelled as follows:

$$\mathbf{T_c^D} = \overline{\rho \mathbf{D_c} \nabla \mathbf{c}} \approx \overline{\rho} \tilde{D}_c \nabla \tilde{c} \tag{A11}$$

$$= (\rho_u (1-\overline{c}) D_u + \rho_b \overline{c} D_b) \nabla \tilde{c} \tag{A12}$$

$$= \left(\rho_u (1-\overline{c}) D_u + \rho_b \overline{c} D_u \frac{T_b^{3/2}}{T_u^{3/2}} \right) \nabla \tilde{c} \tag{A13}$$

$$= \left(\rho_u (1-\overline{c}) D_u + \rho_b \overline{c} D_u \Theta^{3/2} \right) \nabla \tilde{c} \tag{A14}$$

$$= \rho_u \frac{\nu}{\mathrm{Pr}} (1 - \overline{c} + \overline{c} \Theta^{1/2}) \nabla \tilde{c} \tag{A15}$$

The divergence of the molecular flux is proportional to the Laplacian operator $\Delta \tilde{c}$. Determination of the Laplacian is difficult, because the local noise of $\overline{c}$ is amplified after taking divergence and gradient of $\tilde{c}$. $\Delta \overline{c}$ is used instead of $\Delta \tilde{c}$ for higher accuracy measurement in the middle of the flame brush. Laplacian $\overline{c}$ can be re-written as Eq. (A16) and fitted with a physically-based polynomial, $k_1 \overline{c}(1-\overline{c})(1-2k_2\overline{c}+k_3\overline{c}^2)$, along $\overline{c}$ in Figure A2. It is similar to a flat flame, but with allowance for skewness in the distribution of $\Delta \overline{c}$. Details of how Eq. (A16) is chosen can be referred to the B.3.

$$\Delta \overline{c} = k_{|\nabla \overline{c}|}^2 \overline{c}(1-\overline{c})(1-2\overline{c}) + \overline{c}(1-\overline{c}) g(\overline{c}) \tag{A16}$$

where $k_{|\nabla \overline{c}|}$ is the factor of fitting $|\nabla \overline{c}|$ with parabolic equations, $g(\overline{c})$ is a function of $\overline{c}$.

Figure A2 shows measured values of $\Delta \overline{c}$ along the streamlines considered before. The values of $\Delta \overline{c}$ are positive along streamlines close to the center of the flame (**N1** and **P1**), whereas negative values appear away from the centerline near the trailing edge of **N2** and **P2**.

A.2 Molecular diffusion term s_D

As shown shortly, the molecular diffusion is negligible compared with the other two terms. Nevertheless, we still present a detailed discussion on the estimates and extrapolation of s_D to the leading edge into a form appropriate for fitting. Starting from the definition of the term, and the approximation in Eq. (A15), we have:

$$\begin{aligned} s_D &= \frac{\nabla \cdot T_c^D}{\overline{\rho} |\nabla \tilde{c}|} \approx \frac{\rho_u}{\overline{\rho}} \frac{\nu}{\mathrm{Sc}} \frac{\nabla \cdot ((1 - \overline{c} + \overline{c}\Theta^{1/2}) \nabla \tilde{c})}{|\nabla \tilde{c}|} \\ &= \frac{\rho_u}{\overline{\rho}} \frac{\nu}{LePr} \left((1 - \overline{c} + \overline{c}\Theta^{1/2}) \frac{\nabla^2 \tilde{c}}{|\nabla \tilde{c}|} + \frac{\nabla \tilde{c} \cdot \nabla (1 - \overline{c} + \overline{c}\Theta^{1/2})}{|\nabla \tilde{c}|} \right) \\ &= \frac{\rho_u}{\overline{\rho}} \frac{\nu}{Pr} \left((1 - \overline{c} + \overline{c}\Theta^{1/2}) \frac{\Delta \tilde{c}}{|\nabla \tilde{c}|} + (\Theta^{1/2} - 1) |\nabla \overline{c}| \right) \end{aligned} \tag{A17}$$

where Δ is the Laplacian operator, $\Delta\tilde{c} = \nabla \cdot \nabla$, Sc is the Schmidt number and is equal to the Prandtl number Pr when Lewis number Le is equal to 1.

Invoking Eq. (B30) into Eq. (A17), we can have s_D as a function of $\Delta\bar{c}$ and $|\nabla\bar{c}|$, which avoids the term containing Favre-averaged terms and can be more easily fitted by experimental measurement.

$$\begin{aligned} s_D &= \frac{\rho_u}{\bar{\rho}}\frac{\nu}{Pr}\left((1-\bar{c}+\bar{c}\Theta^{1/2})\frac{1}{|\nabla\tilde{c}|}\frac{\rho_u\rho_b}{\bar{\rho}^2}\left(\Delta\bar{c}-\frac{2(\frac{1}{\Theta}-1)}{1+\bar{c}(\frac{1}{\Theta}-1)}|\nabla\bar{c}|^2\right)+(\Theta^{1/2}-1)|\nabla\bar{c}|\right) \\ &= \frac{\rho_u}{\bar{\rho}}\frac{\nu}{Pr}\left((1-\bar{c}+\bar{c}\Theta^{1/2})\frac{\Delta\bar{c}}{|\nabla\bar{c}|}+\left(\Theta^{1/2}-1+\frac{2(1-\frac{1}{\Theta})(1-\bar{c}+\bar{c}\Theta^{1/2})}{1+\bar{c}(\frac{1}{\Theta}-1)}\right)|\nabla\bar{c}|\right) \end{aligned} \tag{A18}$$

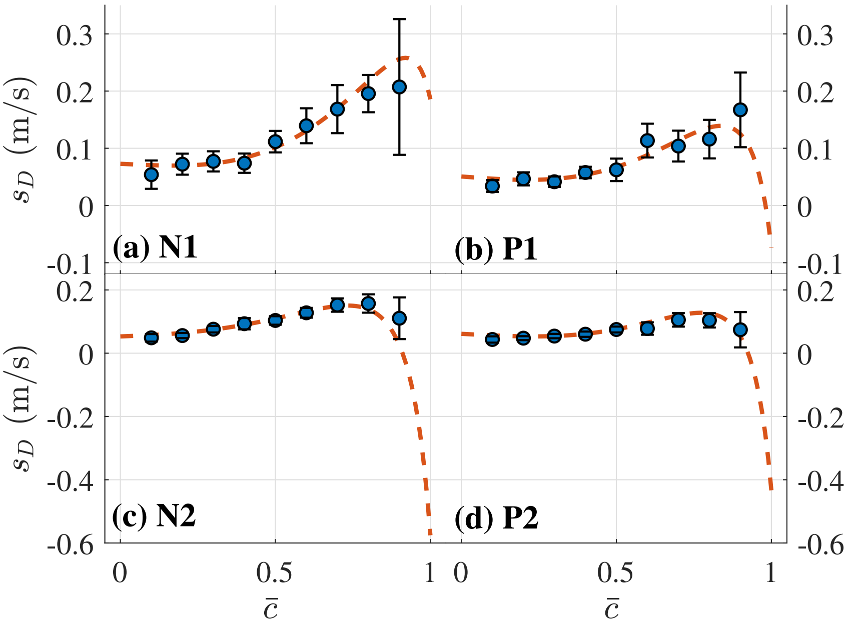

Fig. A3 Molecular diffusion term s_D along streamlines. Blue symbols: measured values, dashed red line: fitted values using Eq. (A18).

Figure A3 shows measured values of s_D and compared fitted results from Eq. (A18). The Laplacian operator $\Delta\bar{c}$ in the first term was fitted with $k_1\bar{c}(1-\bar{c})(1-2k_2\bar{c}+k_3\bar{c}^2))$ in Figure A2.

At both $\bar{c}=0$ and $\bar{c}=1$, the second term in Eq. (A18) is equal to zero, and only the Laplacian term, which is apparently non-zero, makes a contribution to s_D. s_D should be proportional to $k_{|\nabla\bar{c}|}$ at $\bar{c}=0$, and $-\Theta^{3/2}k_{|\nabla\bar{c}|}$ at $\bar{c}=1$, while the actual value depends on fitting results of $\Delta\bar{c}$. The fitted results at the leading edge ($0<\bar{c}<0.1$)

show less uncertainty, while the fitted results in the trailing edge (0.9< $\overline{c}$ <1) are not. However, comparisons with terms Fig. 12 and Fig. 14 show that s_D are of smaller order and can be neglected at current levels of turbulence. Eq. (A18) provides an approach to filter the noise of directly calculating values of s_D and fit the s_D to the leading edge with a reasonable form.

Appendix B Mathematical derivations

B.1 Relationships between Ensemble- and Favre-average quantities based on the flamelet assumption

Conversions between ensemble-averaged variables and density- (or Favre-) averaged variables are useful. Details of the derivations from $\nabla\tilde{c}$ to $\nabla\overline{c}$, and the conversion from $\Delta\tilde{c}$ to $\Delta\overline{c}$ are as follows:

Under the bimodal probability model of the probability distribution function for c, we have

$$\overline{\rho} = \rho_u(1-\overline{c}) + \rho_b\overline{c} \tag{B19}$$

$$\frac{\overline{\rho}}{\rho_u} = \left(1+\overline{c}\left(\frac{1}{\Theta}-1\right)\right) \tag{B20}$$

$$\tilde{c} = \overline{c}\left(\Theta+\overline{c}\left(1-\Theta\right)\right)^{-1} \tag{B21}$$

where $\Theta = \rho_u/\rho_b$, and the densities are reckoned at the corresponding equilibrium equivalence ratios.

To connect $|\nabla\tilde{c}|$ to $|\nabla\overline{c}|$, we start from the gradient of the product $\overline{\rho}\tilde{c} = \rho_b\overline{c}$:

$$\nabla(\overline{\rho}\tilde{c}) = \overline{\rho}\nabla\tilde{c} + \tilde{c}\nabla\overline{\rho} = \rho_b\nabla\overline{c} \tag{B22}$$

$$\begin{aligned}\nabla\tilde{c} &= \frac{\rho_b}{\overline{\rho}}\nabla\overline{c} - \frac{\rho_b\overline{c}}{\overline{\rho}^2}\nabla\overline{\rho} \\ &= \left(1-\overline{c}\frac{\rho_b-\rho_u}{\overline{\rho}}\right)\frac{\rho_b}{\overline{\rho}}\nabla\overline{c} \\ &= \frac{\rho_u\rho_b}{\overline{\rho}^2}\nabla\overline{c}\end{aligned} \tag{B23}$$

The flux term $\widetilde{\mathbf{u}''c''}$, is expressed in terms of the express the conditional velocities, $\overline{\mathbf{u}}_u$ and $\overline{\mathbf{u}}_b$, in order to avoid measurement error in experiments. The following terms come into the equations:

$$\overline{\rho}\tilde{\mathbf{u}} = \overline{\rho\mathbf{u}} = \rho_u(1-\overline{c})\overline{\mathbf{u}}_u + \rho_b\overline{c}\overline{\mathbf{u}}_b \tag{B24}$$

$$(\rho_u(1-\overline{c}) + \rho_b\overline{c})\tilde{\mathbf{u}} = \rho_u(1-\overline{c})\overline{\mathbf{u}}_u + \rho_b\overline{c}\overline{\mathbf{u}}_b \tag{B25}$$

$$\rho_b\overline{c}(\tilde{\mathbf{u}}-\overline{\mathbf{u}}_b) = \rho_u(1-\overline{c})(\overline{\mathbf{u}}_u-\tilde{\mathbf{u}}) \tag{B26}$$

Finally, the Laplacian $\Delta\bar{c}$ can be connected with $\Delta\tilde{c}$ and provides an approach to convert $\Delta\tilde{c}$ into a function of $\Delta\bar{c}$ and $|\nabla\bar{c}|$, which can be more easily fitted.

$$\nabla^2\bar{c} = \nabla\cdot\nabla\bar{c} = \nabla\cdot(\bar{\rho}^2\frac{\nabla\tilde{c}}{\bar{\rho}^2}) = \nabla(\bar{\rho}^2)\cdot\frac{\nabla\tilde{c}}{\bar{\rho}^2} + \frac{\bar{\rho}^2}{\rho_u\rho_b}(\nabla\cdot(\frac{\rho_u\rho_b\nabla\tilde{c}}{\bar{\rho}^2})) \tag{B27}$$

$$= \nabla\left((1+\bar{c}(\frac{1}{\Theta}-1))^2\right)\cdot\frac{\nabla\bar{c}}{(1+\bar{c}(\frac{1}{\Theta}-1))^2} + \frac{\bar{\rho}^2}{\rho_u\rho_b}\nabla\cdot\nabla\tilde{c} \tag{B28}$$

$$= \frac{2(\frac{1}{\Theta}-1)}{1+\bar{c}(\frac{1}{\Theta}-1)}|\nabla\bar{c}|^2 + \frac{\bar{\rho}^2}{\rho_u\rho_b}\Delta\tilde{c} \tag{B29}$$

Finally, we have Laplacian $\Delta\tilde{c}$ as

$$\Delta\tilde{c} = \frac{\rho_u\rho_b}{\bar{\rho}^2}\left(\Delta\bar{c} - \frac{2(\frac{1}{\Theta}-1)}{1+\bar{c}(\frac{1}{\Theta}-1)}|\nabla\bar{c}|^2\right) \tag{B30}$$

B.2 Mathematical derivation of flame surface density

In this Appendix, we show the equivalence between the flame surface definition $\Sigma = |\nabla c\,\delta(c-c^*)|$ and $\Sigma_{\mathrm{A/V}}$ as derived from the zero limits of mean area per volume,

$$\Sigma_{(\mathrm{A/V})} = \frac{1}{N_f}\sum_{i=1}^{N_f}\frac{A_i(\bar{c})}{V(\bar{c})} \tag{B31}$$

B.2.1 Conversion of definitions

To conduct the conversion from Σ to $\Sigma_{(\mathrm{A/V})}$, we define as an infinitesimal volume $dV = dV_u + dV_b$. dV_u and dV_b are volumes of reactant and product in the volume dV, separated by a boundary dA_i.

$$\begin{aligned}\Sigma(\mathbf{x}) &= \lim_{dV\to 0}\frac{1}{dV}\iiint_{dV}\Sigma(\mathbf{x})\,dV \\ &= \lim_{dV\to 0}\frac{1}{dV}\left(\lim_{N_f\to\infty}\frac{1}{N_f}\left(\sum_{1}^{N_f}\iiint_{dV}\Sigma'(\mathbf{x})\,dV\right)\right) \\ &= \lim_{N_f\to\infty}\frac{1}{N_f}\left(\lim_{dV\to 0}\left(\sum_{1}^{N_f}\frac{\iiint_{dV}\Sigma'(\mathbf{x})\,dV}{dV}\right)\right)\end{aligned} \tag{B32}$$

Next, we need to prove the volume integral of Σ' in Eq. (B32) is equal to the total flame surface area dA_i inside any volume. The volume integral in Eq. B32 can be separated into integrals over reactant and product sides.

$$\iiint_{dV}\Sigma'(\mathbf{x})\,dV = \iiint_{dV_b}\Sigma'(\mathbf{x})\,dV + \iiint_{dV_u}\Sigma'(\mathbf{x})\,dV \tag{B33}$$

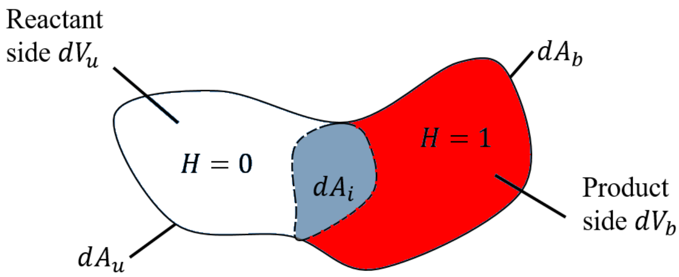

Fig. B4 Illustration of an steady arbitrary infinitesimal volume connecting burned (dV_u) and unburnt (dV_u) volumes, such that $dV = dV_u + dV_b$. The grey surface of area dA_i connects burned, and unburnt regions (in 3D); the areas dA_u and dA_b connect with dA_i to close their respective volumes.

In order to determine the gradient ∇c, the Heaviside function $H(c - c^*) = c\,\delta(c - c^*)$ is used, in the following proof, and H defined in the volume dV. The definition of H at the flame surface is irrelevant to the following proof and can be defined as any value between 0 to 1. In this study, H can be defined as $H_f = 1/2$ on the flame surface where $H(\mathbf{x})$ is discontinuous Abramowitz and Stegun (1964).

$$H = \begin{cases} 0, \ \mathbf{x} \in & \text{reactant} \\ H_f, \ \mathbf{x} \in & \text{flame surface} \\ 1, \ \mathbf{x} \in & \text{product} \end{cases} \tag{B34}$$

Invoking the definition of H and the divergence theorem (twice) into each term on the RHS of Eq. (B33), we have

$$\begin{aligned}
\iiint_{dV_b} \Sigma'(\mathbf{x})\, dV &= \iiint_{dV_b} |\nabla H|\, dV \qquad \text{(B35)} \\
&= \iiint_{dV_b} \frac{\nabla H}{|\nabla H|} \cdot \nabla H\, dV \\
&= \oiint_{dA_i + dA_b} \left(\frac{\nabla H}{|\nabla H|} H \right) \cdot \hat{\mathbf{n}}\, dA - \iiint_{dV_b} H \left(\nabla \cdot \frac{\nabla H}{|\nabla H|} \right) dV \\
&= \oiint_{dA_i} H_f \left(\frac{\nabla H}{|\nabla H|} \right) \cdot \left(- \frac{\nabla H}{|\nabla H|} \right) dA - \iiint_{dV_b} \frac{1}{|\nabla H|} (\nabla \cdot \nabla H)\, dV \\
&= -H_f\, dA_i - \oiint_{dA_i} \frac{1}{|\nabla H|} \nabla H \cdot \hat{\mathbf{n}}\, dA \\
&= -H_f\, dA_i - \oiint_{dA_i} \frac{1}{|\nabla H|} \nabla H \cdot \left(- \frac{\nabla H}{|\nabla H|} \right) dA \\
&= (1 - H_f)\, dA_i \qquad \text{(B36)}
\end{aligned}$$

The same derivation can be conducted on the integral over dV_u, so that,

$$\begin{aligned}
\iiint_{dV_u} \Sigma'(\mathbf{x}) dV &= \iiint_{dV_u} |\nabla H| \, dV \qquad \text{(B37)}\\
&= \iiint_{dV_u} \frac{\nabla H}{|\nabla H|} \cdot \nabla H \, dV \\
&= \oiint_{dA_i+dA_u} \left(\frac{\nabla H}{|\nabla H|} H \right) \cdot \hat{\mathbf{n}} \, dA - \iiint_{dV_u} H \left(\nabla \cdot \frac{\nabla H}{|\nabla H|} \right) \, dV \\
&= \oiint_{dA_i} H_f \left(\frac{\nabla H}{|\nabla H|} \right) \cdot \left(\frac{\nabla H}{|\nabla H|} \right) \, dA \\
&= H_f \, dA_i \qquad \text{(B38)}
\end{aligned}$$

where dA_u is the part of the enclosed surface of dV that encloses dV_u.

The sum of the two equations above yields the LHS of Eq. (B33) as equal to dA_i. Therefore, $\Sigma(\mathbf{x})$ is equivalent to the definition of Σ_{3Dre} based on area per volume.

$$\iiint_{dV} \Sigma'(\mathbf{x}) \, dV = dA_i \qquad \text{(B39)}$$

$$\Sigma(\mathbf{x}) = \lim_{N_f \to \infty} \frac{1}{N_f} \left(\sum_{i=1}^{N_f} \left(\lim_{dV \to 0} \frac{dA_i}{dV} \right) \right) \qquad \text{(B40)}$$

$$\approx \frac{1}{N_f} \left(\sum_{i=1}^{N_f} \frac{dA_i}{dV} \right) = \Sigma_{(\mathrm{A/V})} \qquad \text{(B41)}$$

Or we can re-write $\Sigma_{\mathrm{A/V}}$ as

$$\Sigma_{(\mathrm{A/V})} = \frac{1}{dV} \iiint_{dV} \Sigma(\mathbf{x}) \, dV \qquad \text{(B42)}$$

Overall, the above derivation shows that different definitions of local flame surface densities in 3D are equivalent. The derivations are of course still valid in 2D, where the limit of A/V becomes a line per unit area.

B.2.2 Σ_{2D} measurement and spatial resolution

The present subsection outlines the determination of Σ_{2D} in Eq. (11).We start with the result from the previous appendix, which showed the equivalence $\Sigma_{\mathrm{A/V}} = \overline{|\nabla c \, \delta(c - c^*)|}$. Therefore, the calculation of the 2D version $\Sigma_{\mathrm{A/V}} = \Sigma_{\mathrm{l/A}}$, where l is the conditional flame length, and A the conditional flame area.

Starting from equation Σ_{2D} is equivalent to the ensemble average of flame length per area at the local pixel. If the flame edge is not coincident with the pixel, the magnitude of the gradient is zero; otherwise, the magnitude of the gradient is equal to the flame length per unit area in the pixel. Because of the limited pixel resolution, there is an uncertainty in flame edge direction.

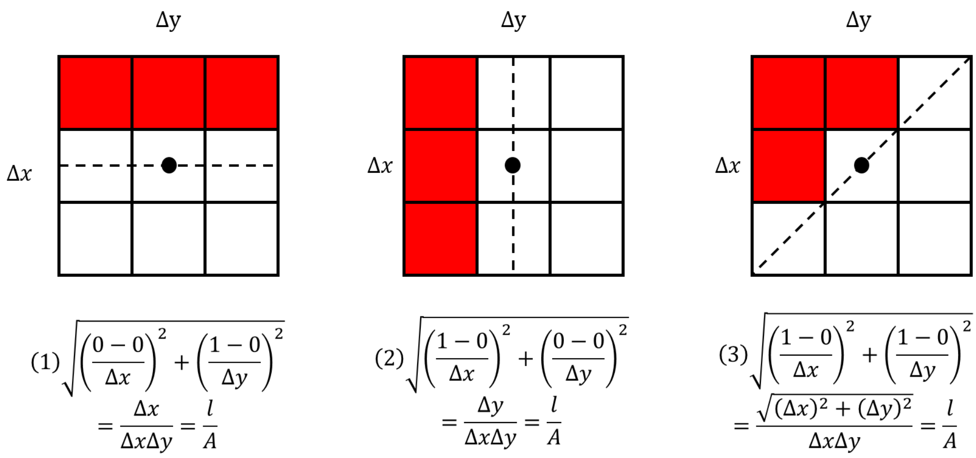

Fig. B5 Illustration of length per area $\sigma_{\mathrm{l/A}}$ in binarized images in each pixel. White: reactant side; Red: product side.

For images with a pixel resolution of Δx mm/pixel $\times$ Δy mm/pixel, the averaged 2D gradient of a binarized image corresponding to an edge pixel can have three different values, shown in Figure B5. Each value represents an approximation of length per area in this pixel. Based on the proof in the last section, $\Sigma_{(\mathrm{A/V})}$ is the spatially-averaged local flame surface Σ in the nearby region, no matter what size the region is. The value of $\Sigma_{2\mathrm{D}}$ derived from the processing method in Eq. (11) also corresponds to a spatially-averaged local flame surface density.

B.3 Modeling the Laplacian operator

The Laplacian $\Delta\bar{c}$ in a 2D field is the divergence of the gradient of $\bar{c}$, and can be rewritten by using an angle form of $\nabla\bar{c}$ as follows:

$$\begin{aligned}\Delta\bar{c} &= \nabla\cdot(|\nabla\bar{c}|\sin\alpha, |\nabla\bar{c}|\cos\alpha) = \frac{\partial}{\partial x}(|\nabla\bar{c}|\sin\alpha) + \frac{\partial}{\partial y}(|\nabla\bar{c}|\cos\alpha)\\ &= \frac{\partial|\nabla\bar{c}|}{\partial x}\sin\alpha + |\nabla\bar{c}|\cos\alpha\frac{\partial\alpha}{\partial x} + \frac{\partial|\nabla\bar{c}|}{\partial y}\cos\alpha - |\nabla\bar{c}|\sin\alpha\frac{\partial\alpha}{\partial y}\end{aligned} \tag{B43}$$

Invoking the parabolic fitting of $|\nabla\bar{c}|$ into Eq. (B43) and considering the variation of α across different streamlines, we can re-write Laplacian $\Delta\bar{c}$ into a polynomial form which must go across zero at $\bar{c}=0$ and $\bar{c}=1$.

$$\Delta\bar{c} = k^2_{|\nabla\bar{c}|}\bar{c}(1-\bar{c})(1-2\bar{c}) + \bar{c}(1-\bar{c})g(\bar{c}) \tag{B44}$$

where $k_{|\nabla\bar{c}|}$ is the factor of fitting $|\nabla\bar{c}|$ with parabolic equations, $g(\bar{c})$ is a function of $\bar{c}$.

The derivation of Eq. (B44) is given as follows. In the present approximation, we assume that (a) there is a field of the mean progress of reaction $\bar{c}$, and that (b) the gradient of the field in the direction of the normal to the flame brush can be represented as $\nabla\bar{c} = k\bar{c}(1-\bar{c})$, where k may be a local constant.

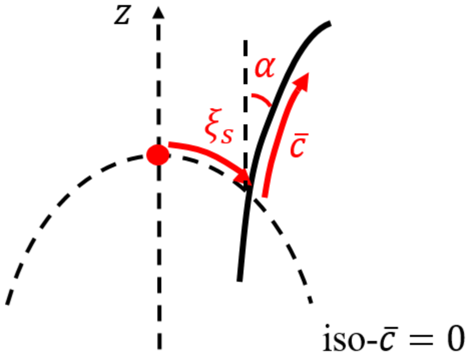

Fig. B6 Illustration of coordinate defined in modeling the Laplacian operator

In a 2D flame, α, the angle between the normal vector $\hat{\mathbf{n}}$ and $z-$axis, can be expressed as a function of $\bar{c}$ and a symbol which represents the selected streamline and can be defined in various ways. Here, we define a ξ_s as the spatial distance along the isocontour $\bar{c}=0$ from the local streamline to the central line ($r=0$) in Figure B6.

Therefore, Eq. (B43) can be expanded as follows:

$$\Delta\bar{c} = \left(k(1-2\bar{c})\frac{\partial\bar{c}}{\partial x} + \bar{c}(1-\bar{c})\frac{\partial k}{\partial x}\right)\sin\alpha + \left(k(1-2\bar{c})\frac{\partial\bar{c}}{\partial y} + \bar{c}(1-\bar{c})\frac{\partial k}{\partial y}\right)\cos\alpha + ...$$
$$|\nabla\bar{c}|\left(\cos\alpha\frac{\partial\alpha}{\partial x} - \sin\alpha\frac{\partial\alpha}{\partial y}\right) \tag{B45}$$
$$=k(1-2\bar{c})\left(\sin\alpha\frac{\partial\bar{c}}{\partial x} + \cos\alpha\frac{\partial\bar{c}}{\partial y}\right) + \bar{c}(1-\bar{c})\left(\sin\alpha\frac{\partial k}{\partial x} + \cos\alpha\frac{\partial k}{\partial y}\right) + ...$$
$$|\nabla\bar{c}|\left(\cos\alpha\left(\frac{\partial\alpha}{\partial\bar{c}}\frac{\partial\bar{c}}{\partial x} + \frac{\partial\alpha}{\partial\xi_s}\frac{\partial\xi_s}{\partial x}\right) - \sin\alpha\left(\frac{\partial\alpha}{\partial\bar{c}}\frac{\partial\bar{c}}{\partial y} + \frac{\partial\alpha}{\partial\xi_s}\frac{\partial\xi_s}{\partial y}\right)\right) \tag{B46}$$
$$=k(1-2\bar{c})\left(\sin^2\alpha|\nabla\bar{c}| + \cos^2\alpha|\nabla\bar{c}|\right) + \bar{c}(1-\bar{c})\left(\sin\alpha\frac{\partial\xi_s}{\partial x} + \cos\alpha\frac{\partial\xi_s}{\partial y}\right)\frac{\partial k}{\partial\xi_s} + ...$$
$$|\nabla\bar{c}|\left(\cos\alpha\left(\frac{\partial\alpha}{\partial\bar{c}}|\nabla\bar{c}|\sin\alpha + \frac{\partial\alpha}{\partial\xi_s}\frac{\partial\xi_s}{\partial x}\right) - \sin\alpha\left(\frac{\partial\alpha}{\partial\bar{c}}|\nabla\bar{c}|\cos\alpha + \frac{\partial\alpha}{\partial\xi_s}\frac{\partial\xi_s}{\partial y}\right)\right) \tag{B47}$$
$$=k^2\bar{c}(1-\bar{c})(1-2\bar{c}) + \bar{c}(1-\bar{c})\left(\left(\sin\alpha\frac{\partial\xi_s}{\partial x} + \cos\alpha\frac{\partial\xi_s}{\partial y}\right)\frac{\partial k}{\partial\xi_s} + k\left(\cos\alpha\frac{\partial\xi_s}{\partial x} - \sin\alpha\frac{\partial\xi_s}{\partial y}\right)\frac{\partial\alpha}{\partial\xi_s}\right) \tag{B48}$$

Based on Figure 5, the variation of α along one streamline is small, and we can approximately assume $\frac{\partial\xi_s}{\partial x} = \cos\alpha_0$ and $\frac{\partial\xi_s}{\partial y} = -\cos\alpha_0$ along each streamline, where

$\alpha_0 = \alpha(\bar{c} = 0, \xi_s)$. Then, Eq. (B48) can be further simplified as

$$\Delta\bar{c} \approx k^2\bar{c}(1-\bar{c})(1-2\bar{c}) + \bar{c}(1-\bar{c})\left(\sin(\alpha-\alpha_0)\frac{\partial k}{\partial \xi_s} + k\cos(\alpha-\alpha_0)\frac{\partial \alpha}{\partial \xi_s}\right) \quad \text{(B49)}$$

$$\approx k^2\bar{c}(1-\bar{c})(1-2\bar{c}) + \bar{c}(1-\bar{c})\left((\alpha-\alpha_0)\frac{\partial k}{\partial \xi_s} + k\frac{\partial \alpha}{\partial \xi_s}\right) \quad \text{(B50)}$$

$$= \bar{c}(1-\bar{c})g(\bar{c}, \xi_s) \quad \text{(B51)}$$

where $g(\bar{c}, \xi_s) = \left(k^2(1-2\bar{c}) + (\alpha-\alpha_0)\frac{\partial k}{\partial \xi_s} + k\frac{\partial \alpha}{\partial \xi_s}\right)$

$\frac{\partial k}{\partial \xi_s}$ only depends on ξ_s and is a constant along each streamlines. $\frac{\partial \alpha}{\partial \xi_s}$ obviously depends on $\bar{c}$ and ξ_s, and can be expressed as a function of $\bar{c}$ along each streamlines. Therefore, the second term in Eq. (B50) can be expressed as a function of $\bar{c}$. To avoid over-fitting and consider a higher-order of $\bar{c}$ in α, $g(\bar{c}, \xi_s)$is considered as a second-order polynomial in each streamline during the fitting process, and we have a final form of fitting Laplacian $\Delta\bar{c}$ as

$$\Delta\bar{c} = k_1\bar{c}(1-\bar{c})(1-2k_2\bar{c}+k_3\bar{c}^2) \quad \text{(B52)}$$