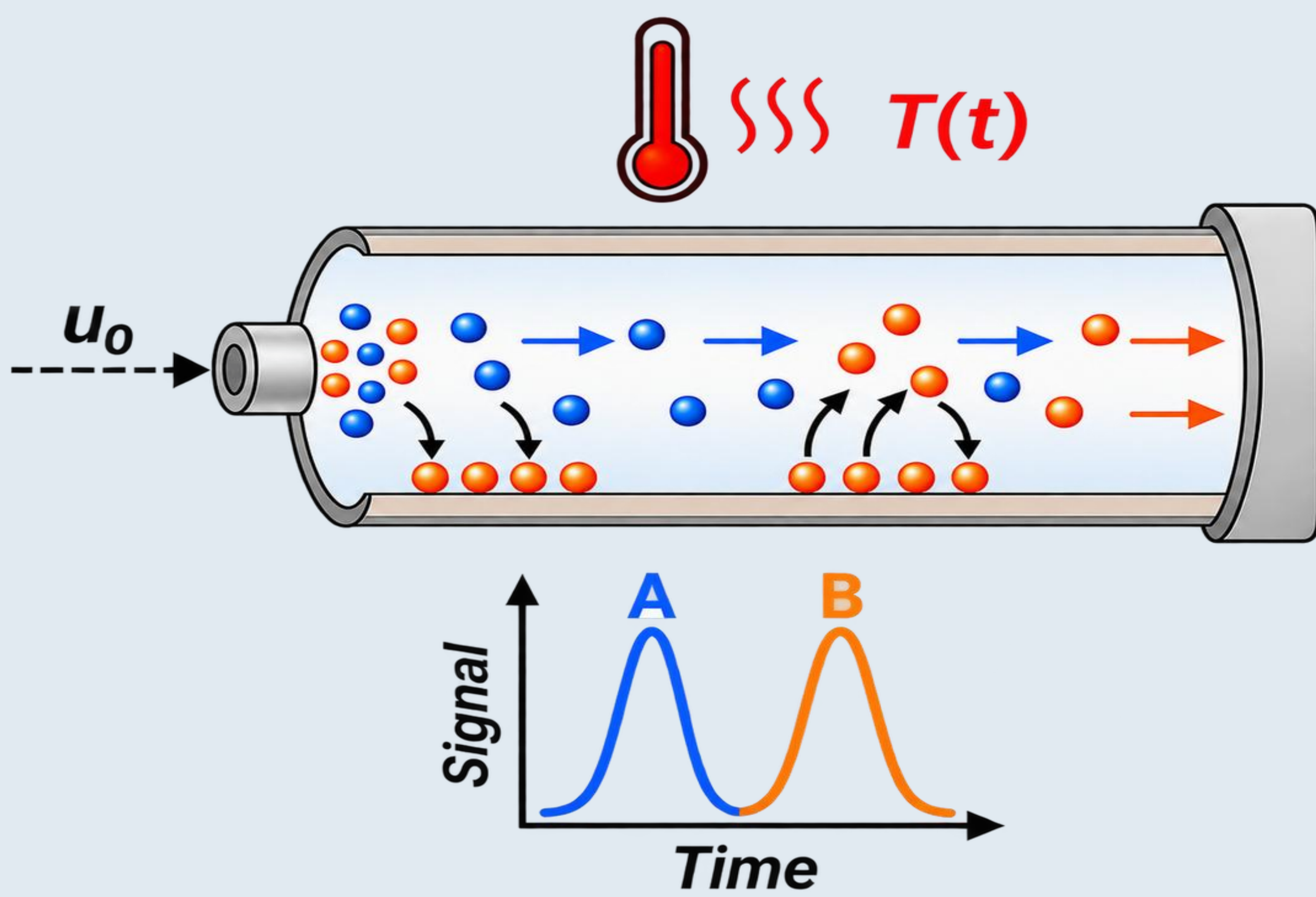


Optimal Control of Gas Chromatography Separation Using a 1D Adsorption-Desorption Model

Control the temporal separation of two gas species by optimizing flow velocity and heating

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Abstract

This work presents a COMSOL Multiphysics® proof of concept for model-based control of gas chromatography separation in a capillary column. A reduced one-dimensional model couples axial advection–diffusion with reversible adsorption at the stationary phase and temperature-dependent desorption described by an Arrhenius law. The carrier-gas velocity and heating transition time are optimized to impose a prescribed outlet delay between two gaseous species. To obtain a robust arrival-time estimate, the retained-species signal is characterized using a weighted temporal barycenter rather than direct peak detection. The resulting

dimensionless cost function is minimized with the derivative-free BOBYQA algorithm by jointly adjusting the carrier-gas velocity and the heating transition time within prescribed bounds. The optimized operating conditions reproduce the prescribed 176 s separation delay with an error of only about 2.9×10^{-3} s. This result shows that the coupled transport–adsorption model can be effectively used to tune chromatographic operating conditions and accurately control the temporal separation of the two species at the detector.

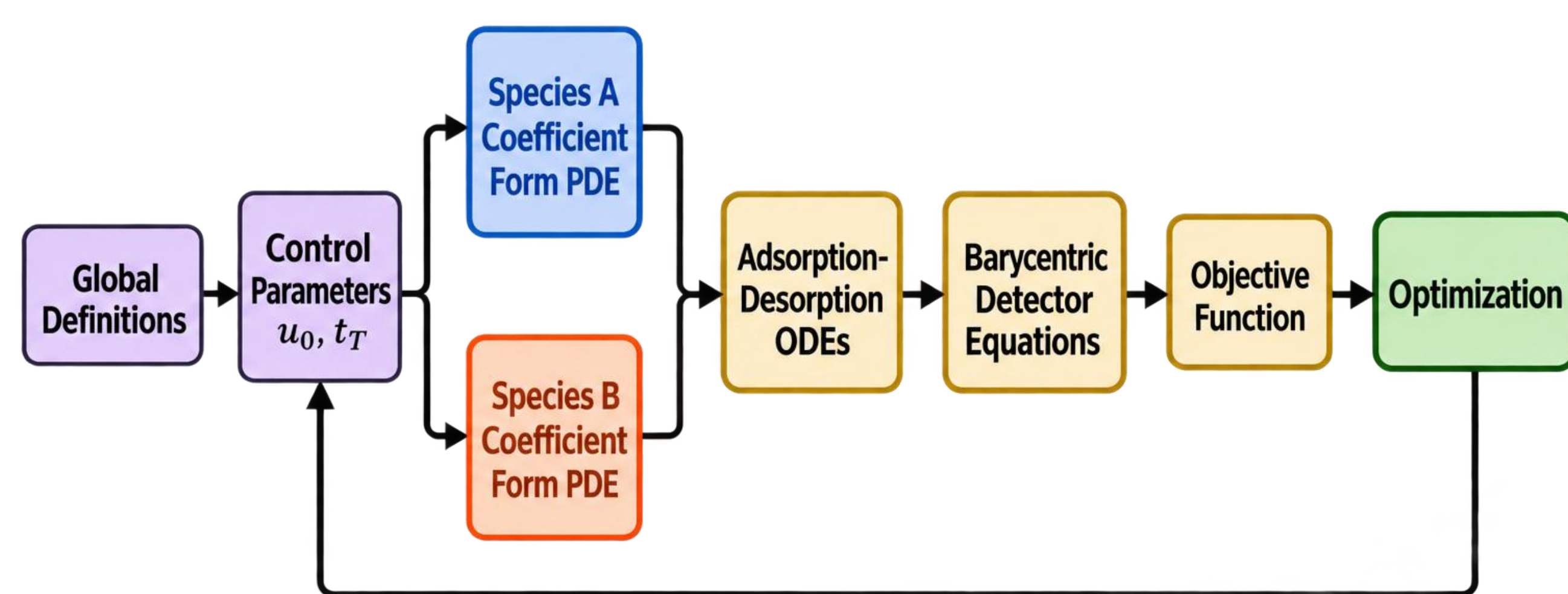


FIGURE 1. COMSOL workflow coupling the 1D transport model, adsorption–desorption kinetics, barycentric outlet detection, and BOBYQA optimization of u_0 and t_T .

Methodology

- 1D Transport Model:** axial advection–diffusion of two gaseous species coupled with reversible adsorption–desorption kinetics at the stationary-phase wall.
- Temperature Control:** desorption rates follow an Arrhenius law, with a smooth temperature ramp controlling the release of the retained species.
- Barycentric Detection:** outlet signals are evaluated at the detector, while the arrival time of species B is estimated from weighted temporal moments.
- Optimization:** BOBYQA adjusts u_0 and t_T within prescribed bounds to minimize the error between the achieved and target outlet delay.

Results

The optimization targets a prescribed delay $\tau = 176$ s between the arrival of species A and the barycentric arrival of species B. The dimensionless cost function is

$$J_{\text{delay}} = \frac{(\hat{t}_B - t_A - \tau)^2}{\tau^2}$$

where $\hat{t}_B$ is the barycentric arrival time of species B and t_A is the reference arrival time of species A. BOBYQA converged after 19 model evaluations. The best parameter pair was $u_0^* = 0.10419$ m s⁻¹ and $t_T^* = 181.58$ s, with $J_{\text{delay}} = 2.6874 \times 10^{-10}$. At the optimized conditions, species A reaches the detector at approximately 288 s, while species B arrives near 464 s. The prescribed 176 s separation is therefore reproduced with an error of only 2.9×10^{-3} s, demonstrating the feasibility of the proposed control strategy.

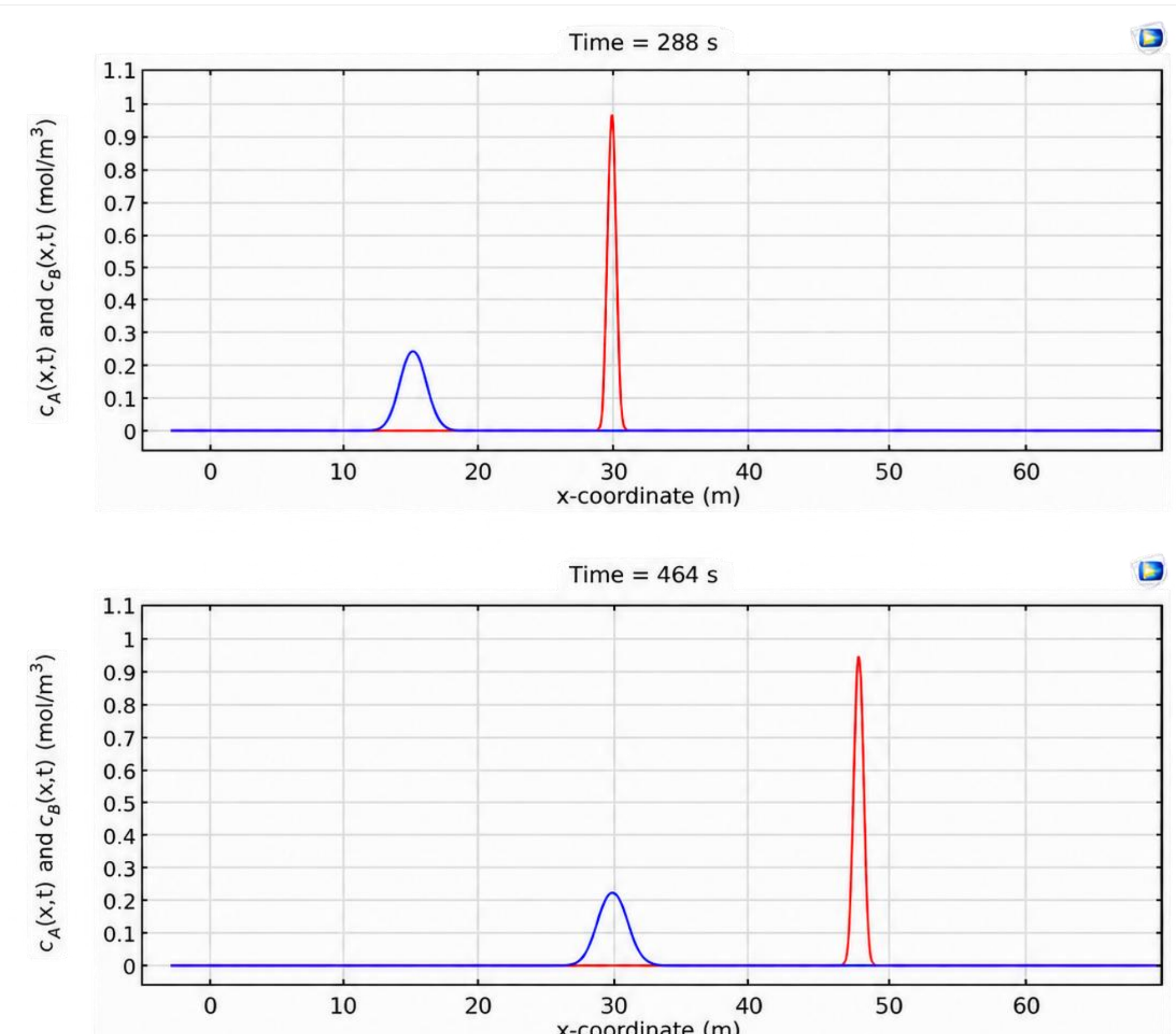


FIGURE 2. Optimized concentration profiles for the 176 s detector delay.

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