Numerical Simulations of Marangoni Convection in an Evaporating Water-Ethanol Mixture Film on a Structured Substrate

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The evaporation of a binary water–ethanol film on a structured, heated substrate is investigated numerically. The wall topography induces a non-uniform distribution of the temperature and composition along the liquid-gas interface. The resulting gradients of surface tension invoke Marangoni convection. We examine the film dynamics and flow pattern evolution during film evaporation.

Motivation and Goal

Motivation

- Evaporation of multicomponent thin films plays an integral role in technologies such as coatings, microelectronics, optoelectronics, and energy devices [1].
- Preferential evaporation leads to interfacial temperature and concentration gradients, generating surface-tension variations driving Marangoni convection.
- Surface topography can be used to control Marangoni convection and surface deformation in liquid films [2].

Goals

- Development of a CFD framework capturing the interaction between long-scale Marangoni convection induced by substrate topography and short-wave Marangoni instability, and to assess their impact on transport in an evaporating binary film.

Method

- An Arbitrary Lagrangian–Eulerian (ALE) framework implemented in COMSOL Multiphysics to resolve the moving liquid–gas interface
- Convective-diffusive mass transport of ethanol in the liquid phase and vapor transport of ethanol and water in the gas phase
- Concentration-dependent thermophysical properties of the binary mixture, with surface tension expressed as a function of mass fraction and temperature [3].
- Evaporation rate of each species is determined by its thermodynamic activity at the interface and its connective-diffusive transport in air

Model Formulation

Governing Equations

- Continuity equation:

$$\nabla \cdot \mathbf{u} = 0 \quad (1)$$

- Navier-Stokes equation:

$$\rho\left(\frac{\partial \boldsymbol{u}}{\partial t} + (\boldsymbol{u}\cdot\nabla)\boldsymbol{u}\right) = \nabla\cdot\left(-\boldsymbol{p} + \mu(\nabla\boldsymbol{u} + \nabla\boldsymbol{u}^T)\right) \quad (2)$$

- Energy equation:

$$\frac{\partial(\rho C_p T)}{\partial t} + \nabla\cdot(\boldsymbol{u}\rho C_p T) = \nabla\cdot(k\nabla T) \quad (3)$$

- Transport of species equation:

$$\frac{\partial C_j}{\partial t} + \nabla\cdot(\boldsymbol{u}C_j) = \nabla\cdot(D_j\nabla C_j) \quad (4)$$

Conditions at the Liquid–Gas Interface

- Thermodynamic equilibrium:

$$C_{sat,i} = \gamma_i x_i p_{sat,i} \quad (5)$$

- Velocity jump:

$$\boldsymbol{u_g} - \boldsymbol{u_l} = \left[(1/\rho_g) - (1/\rho_l)\right](-J_e - J_w)\boldsymbol{n} \quad (6)$$

- Normal Stress Balance:)

$$(\boldsymbol{n}\cdot\tau_g - \boldsymbol{n}\cdot\tau_l)\cdot\boldsymbol{n} = \frac{\sigma}{r_c}\cdot\boldsymbol{n} \quad (7)$$

- Tangential Stress Balance:

$$(\boldsymbol{n}\cdot\tau_g - \boldsymbol{n}\cdot\tau_l)\cdot\boldsymbol{t} = -\sigma_T\nabla_s T - \sigma_c\nabla_s c \quad (8)$$

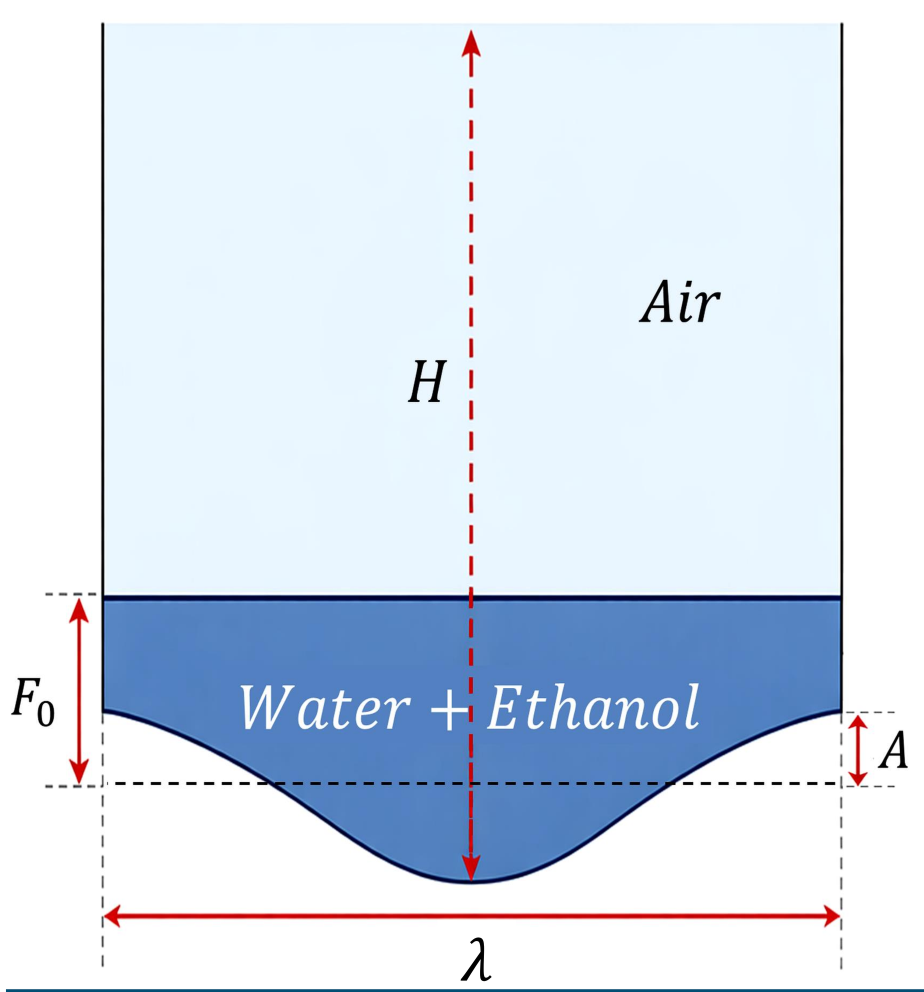
- Energy balance incorporating cooling

$$\boldsymbol{n}\cdot\left(k_g(\nabla T)_g - k_l(\nabla T)_l\right) = -J_e L_e - J_w L_w \quad (9)$$

- Moving interface kinematic condition

$$\boldsymbol{u}_{mesh} = (\boldsymbol{u_l}\cdot\boldsymbol{n} - (J_e + J_w)/\rho_l)\boldsymbol{n} \quad (10)$$

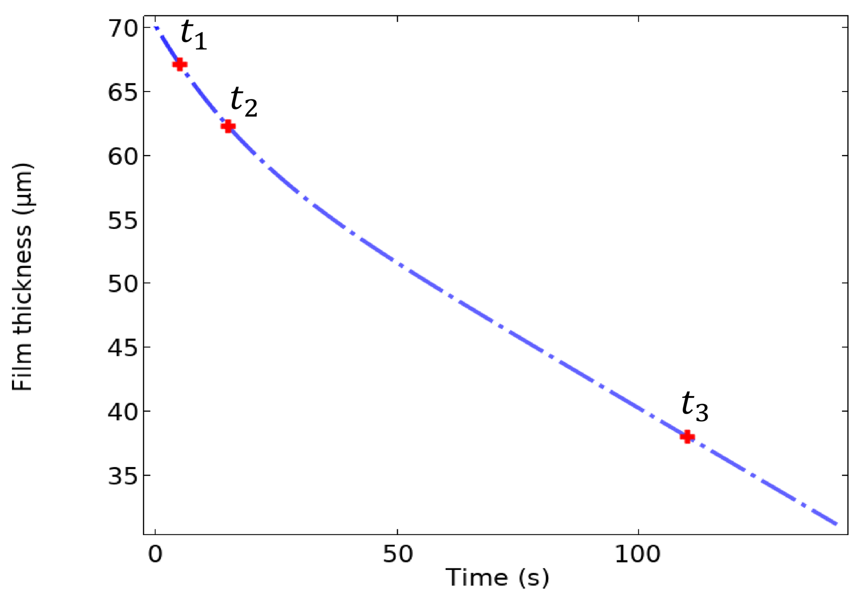
Geometry



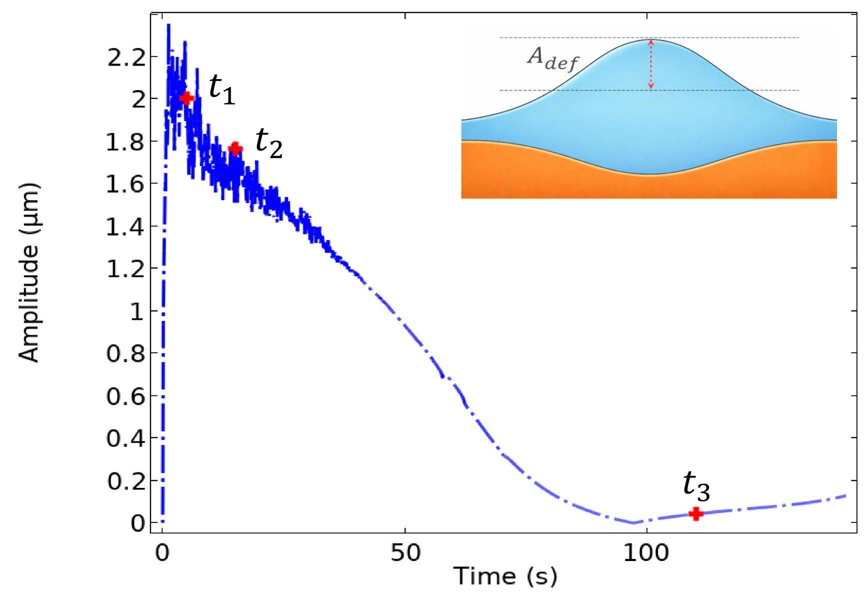
Parameters

A	10 $[\mu m]$	Substrate wave amplitude
F_0	70 $[\mu m]$	Initial film thickness
H	2 $[mm]$	Domain height
λ	1 $[mm]$	Wave length of substrate
T_0	293.15 $[K]$	Initial temperature
ΔT	10 $[K]$	Substrate heating
ξ_0	16.9 [%]	Initial mass fraction of ethanol

Results: Interface Shrinkage and Deformation

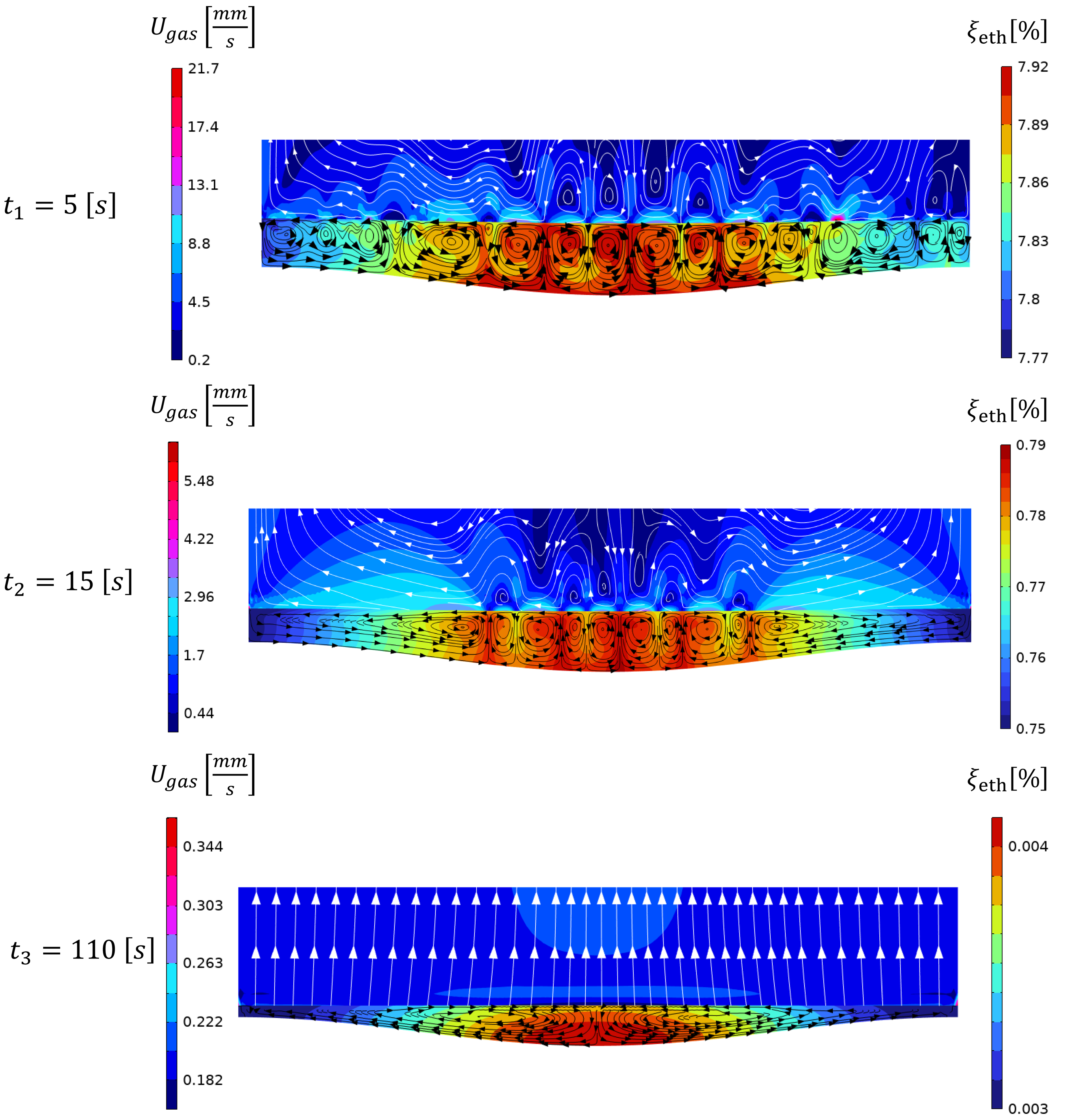


Average film thickness



Amplitude of film interface deformation

Results: Ethanol Distribution and Flow Structure



Conclusions

- Chaotic interface deformations and a high evaporation rate are initially observed; both diminish as the concentration of the more volatile ethanol component decreases.
- At early times, ethanol-rich conditions trigger strong solutal Marangoni instabilities, generating short-wavelength vortices with highly localized velocity fields.
- As ethanol depletes, the solutal influence weakens and the system transitions to a more stable regime dominated by thermal Marangoni convection in the water-rich film, characterized by two large counter-rotating vortices and a reduction in velocity.

References

[1] A. P. Arun et al., Processes 13, 3846 (2025).
[2] Y. O. Kabova et al., Phys. Fluids 18, 012104 (2006).
[3] I. S. Khattab et al., Korean J. Chem. Eng. 29, 812–817 (2012).

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