One-dimensional Spray Combustion Optimization with a Sequential Linear Quadratic Algorithm

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- **Develop a framework for optimal control of continuous combustor**
- **Optimize distribution of secondary air addition to spray combustor**
- **Consider steady, one-dimensional spray combustion model**
- **Formulate ODEs accounting for droplet heating, vaporization, and acceleration; air addition; vapor-air mixing; exothermic oxidation**
- **Apply the Sequential Linear Quadratic (SLQ) Algorithm of Sideris & Bobrow with rate of air addition per increment of length as the control variable.**

Three combustion models were used for optimization:

- **Vaporization – Mixing – Reaction Model. Seven characteristic rates or time: gas residence, droplet residence (or lifetime), droplet heating rate, vaporization rate, droplet acceleration, vapor / air -mixing rate, and oxidation rate.**
- **Vaporization - Mixing Model. Six characteristic rates: oxidation occurs upon mixing.**
- **Vaporization Model. Five characteristic rates: mixing and oxidation occur upon vaporization.**

All models have the rate of secondary-air addition as a control variable. All rates can have multi-time scales.

The targets of the optimization process are to have a prescribed amount of total air addition with complete vaporization and burning of the fuel within the prescribed length.

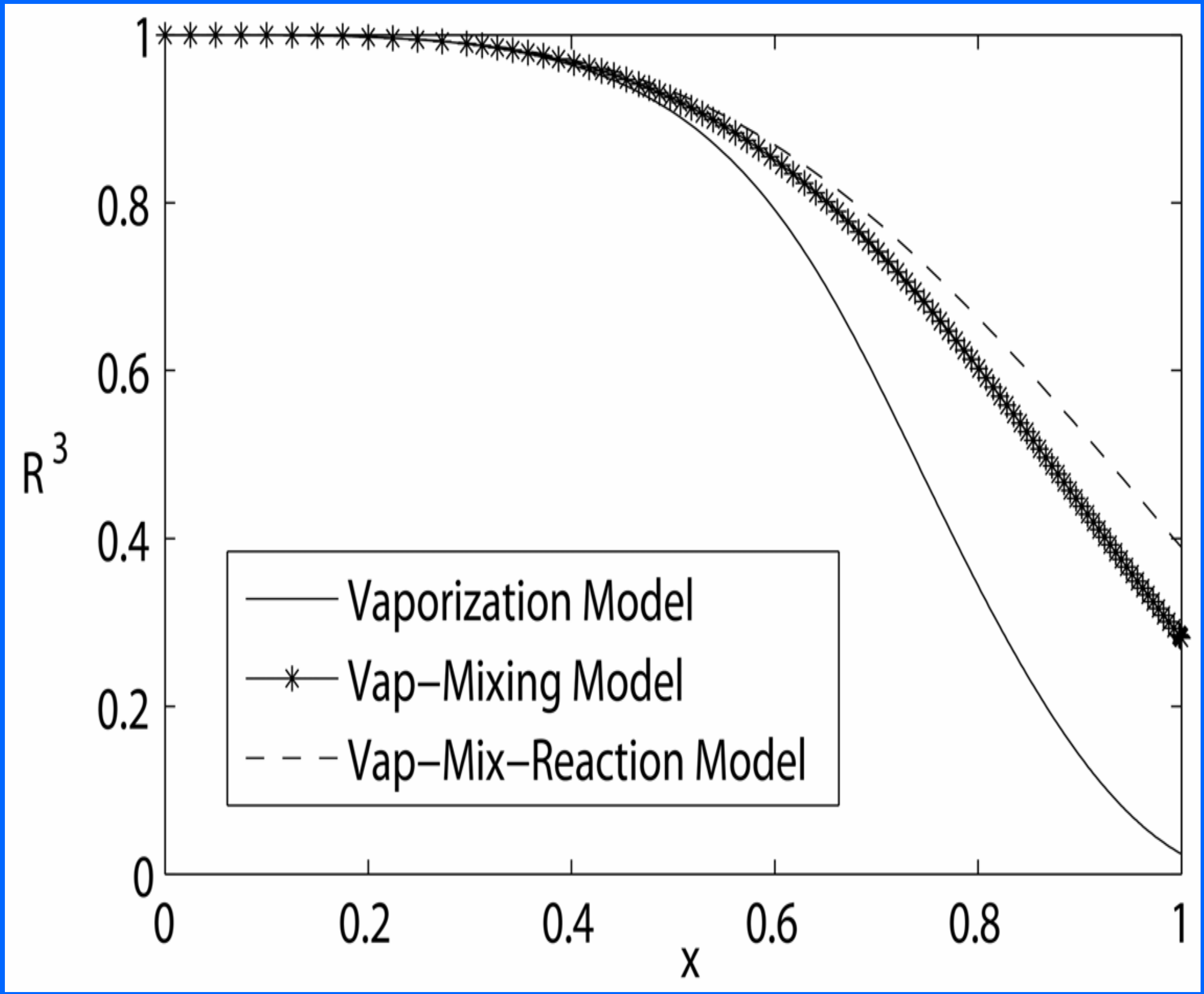
The net effect of air addition is not obvious; it accelerates gas and droplet, decreasing residence time; cools gas, slowing vaporization; increases relative gas-drop velocity, increasing vaporization rate.

$$\mathbf{z} = \frac{d}{dx}\begin{pmatrix} R^3 \\ R^3 u_l \\ R^3 T_l \\ u_g \\ T_g \\ Y_F \\ Y_O \\ m_a \end{pmatrix} = \frac{d}{dx}\begin{pmatrix} z_1 \\ z_2 \\ z_3 \\ z_4 \\ z_5 \\ z_6 \\ z_7 \\ z_8 \end{pmatrix}$$

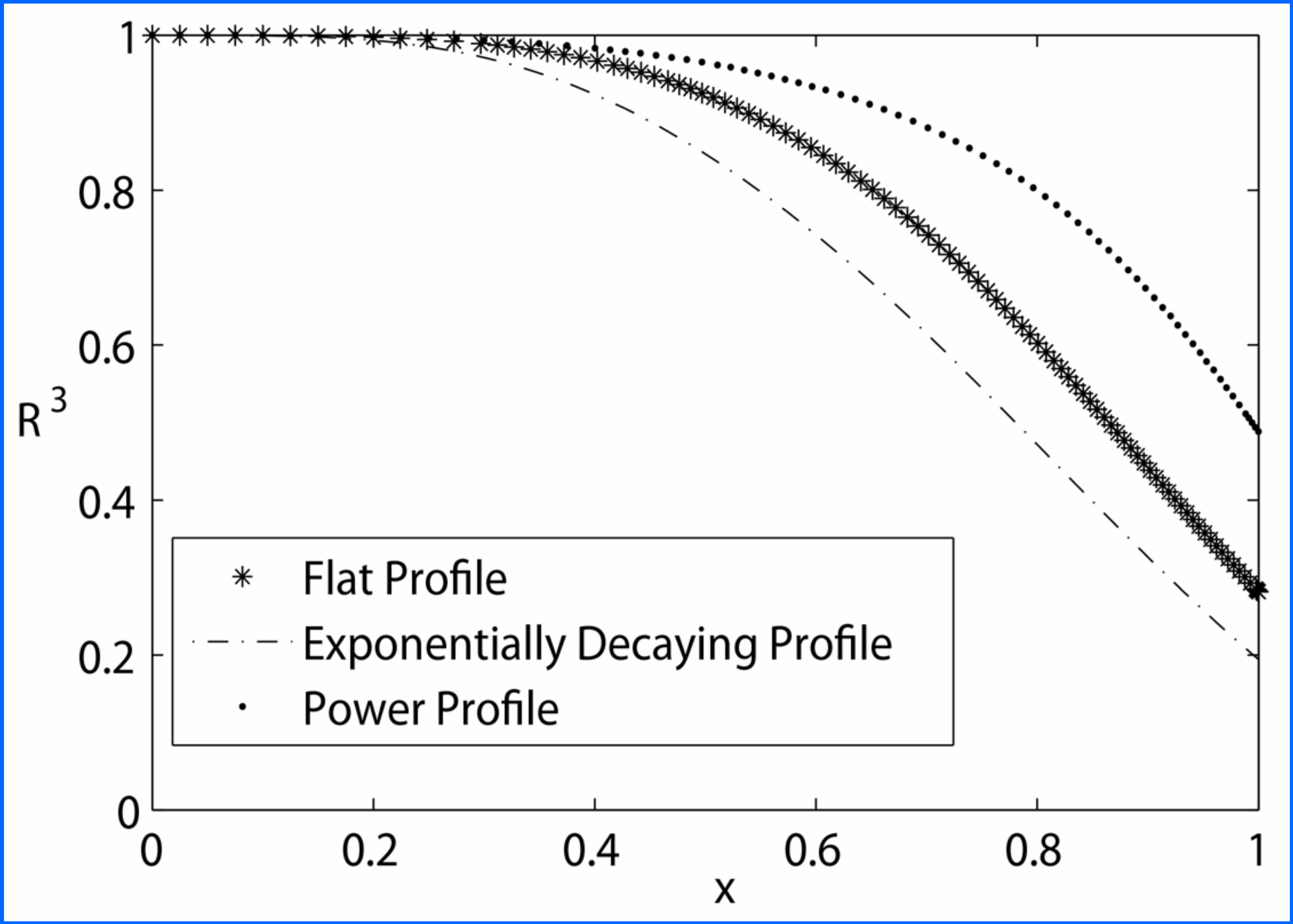
$$= \begin{pmatrix} -\frac{\tilde{\mu}\dot{M}}{u_{l0}} \\ \frac{\tilde{\mu}}{u_{l0}}[D - \dot{M} z_2/z_1] \\ \frac{\tilde{\mu}\dot{M}}{u_{l0}}[\frac{c_p}{c_{v_l}} L_{eff} - \frac{R^*}{c_{v_l}} La - z_3/z_1] \\ \frac{d\dot{m}_a}{dx} - \dot{M} L_{eff} + \kappa Q z_6 \\ \frac{z_5}{z_4}(1 - z_5)\frac{d\dot{m}_a}{dx} - \frac{z_5}{z_4}\dot{M}(L_{eff} + z_5) \\ +\kappa Q z_6 \\ \frac{z_5}{z_4}\dot{M}(1 - z_6) - \frac{z_5}{z_4}\frac{d\dot{m}_a}{dx} z_6 - \kappa z_6 \\ \frac{z_5}{z_4}\frac{d\dot{m}_a}{dx}(1 - z_7) - \frac{z_5}{z_4}\dot{M} z_7 - \kappa \frac{z_6}{\nu} \\ U^2 \end{pmatrix}$$

Based on conservation principles, ODEs govern drop radius, velocity , temperature; gas velocity, temperature; mass fractions of fuel vapor and oxygen; mass flux of secondary air as a function of downstream position.

Source terms on RHS result from vaporization, droplet heating, droplet drag, gas mixing, air addition, exothermic reaction, and gas expansion



Results without optimization for nondimensional droplet volume versus downstream position in combustor: obviously, models which assume some rates are infinite result in faster vaporization and burning.



Three profiles are prescribed which distribute secondary air addition differently with Vaporization-Mixing model: exponential adds most air in upstream portion before mid-length position; power profile adds most air downstream; flat profile has uniform distribution. With optimization process, the profile is determined not prescribed.

OPTIMIZATION METHOD

- The nonlinear system of ODEs are solved numerically with a dependence on the control variable U.

$$\dot{\mathbf{z}}(x) = \mathbf{f}(\mathbf{z}(x), U(x)); \quad \mathbf{z}(0) = \mathbf{z}_0$$

- Target values at the exit are set in a consistent manner.

$$\mathbf{z}_t(x=1) = \left[0 \;\; na \;\; na \;\; na \;\; T_e \;\; 0 \;\; na \;\; \frac{\dot{m}_1^*}{\dot{m}_0^*} \right]$$

- A cost function J is created in both a continuous and a discrete form.

$$J = \Phi(\mathbf{z}(x=1)) + \int_0^1 l(\mathbf{z}(x), U(x))dx$$

$$\min_U \;\; J = \Phi(\mathbf{z}(N)) + \sum_{n=0}^{N-1} L(\mathbf{z}(n), U(n), n)$$

- Finite differencing creates a relationship between adjacent discrete values.

$$\mathbf{z}(n+1) = \mathbf{F}(\mathbf{z}(n), U(n)); \quad \mathbf{z}(0) = \mathbf{z}_0$$

- A quadratic form is taken for the cost function. It can account for exit values as well as interior values. We used only exit values here.

$$L(\mathbf{z}(n), U(n), n) = \frac{1}{2}[\mathbf{z}(n) - \mathbf{z}_t(n)]^T \mathbf{Q}(n)[\mathbf{z}(n) - \mathbf{z}_t(n)] + \frac{1}{2}[U(n) - U_t(n)]^T P(n)[U(n) - U_t(n)]$$

$$\Phi(z) = \frac{1}{2}[\mathbf{z} - \mathbf{z}_t(N)]^T \mathbf{Q}(N)[\mathbf{z} - \mathbf{z}_t(N)]$$

- Weighting factors are prescribed for the contribution of each exit value to the cost function.

$$\mathbf{Q}_t(x=1) = (10^4\ 0\ 0\ 0\ 10^4\ 10^4\ 0\ 10^4)^T$$

Step 0: Provide initial guess for the control (typically zero)

Step 1: Simulate Nonlinear Dynamic Equations and obtain state trajectory

Step 2: Linearize the nonlinear system dynamics about $z_m = [\, z^T(0), z^T(1), \ldots, z^T(n), \ldots, z^T(N) \,]^T$ and $U_m = [\, U(0), U(1), \ldots, U(n), \ldots, U(N-1)]^T$; subscript m indicates the iteration step.

$$\mathbf{F}_z = \frac{\partial \mathbf{F}}{\partial z} \text{ and } \mathbf{F}_U = \frac{\partial \mathbf{F}}{\partial U}$$

$$\bar{\mathbf{z}}(n+1) = \mathbf{F}_z(\mathbf{z}(n), U(n))\bar{\mathbf{z}}(n) + \mathbf{F}_U(\mathbf{z}(n), U(n))\bar{U}(n) \qquad \bar{\mathbf{z}}(0) = 0.$$

The overbar indicates the linearized variable.

Now, solve the Linear Quadratic (LQ) optimal control for the cost function subject to linearized dynamics, using established methods. This does not immediately give the optimal control for the nonlinear problem. Iteration to a converged solution is required.

Step 3: Use the solution U_m of the previous LQ sub problem as a search direction and compute the next control:

$$\mathbf{U}_{m+1} = \mathbf{U}_m + \alpha_m \cdot \bar{\mathbf{U}}_m \qquad \min_{\alpha_m > 0} J[U_m + \alpha_m \cdot \bar{U}_m]$$

The linearization about the previous solution in the iteration requires the use of gradients of all terms on the RHS of the ODEs with respect to each of the independent variables.

$$\begin{pmatrix} f_1(x,u) \\ f_2(x,u) \\ f_3(x,u) \\ f_4(x,u) \\ f_5(x,u) \\ f_6(x,u) \end{pmatrix} = \begin{pmatrix} -\dot{M}\frac{\tilde{\mu}}{u_{l0}} \\ \frac{D\tilde{\mu}}{u_{l0}} - z_2\dot{M}\frac{\tilde{\mu}}{z_1 u_{l0}} \\ \frac{\tilde{\mu}}{u_{l0}}\dot{M}(gz_1^{1/3} - \frac{z_3}{z_1^{2/3}}) \\ w + \dot{M}q \\ z_5(1-z_5)w + \dot{M}\frac{q-z_5}{z_4} \\ w \end{pmatrix}$$

we defined:

$$\begin{aligned} q &= \frac{Q^*}{c_p T_a} - L_{eff} \\ g &= \frac{c_p}{c_{v_l}} L_{eff} - \frac{R^*}{c_{v_l}} \\ \dot{M} &= 4\pi c_1 \sigma_1 \sigma_2 \frac{z_1}{z_2} ln(1+B)h \\ w &= U^2. \end{aligned}$$

Examples of gradient terms but not a complete list.

$$\frac{\partial f_1}{\partial z_1} = -\frac{\partial \dot{M}}{\partial z_1}\frac{\tilde{\mu}}{u_{l0}}$$

$$\frac{\partial D}{\partial z_4} = 6\sigma_1\pi c_1 \frac{z_1^{4/3}}{(1+B)z_2}\frac{|z_4 - \frac{z_2}{z_1}|}{z_4 - \frac{z_2}{z_1}}$$

$$\frac{\partial \dot{M}}{\partial z_2} = 4\sigma_1\sigma_2\pi c_1 ln(1+B)\frac{-z_1^{4/3}}{z_2^2}[\frac{-z_1^{4/3}}{z_2^2}(1 + (Re/2)e^{-Re} + .42\frac{Re^{1/2}}{F}(1-e^{-Re})) + \frac{z_1^{4/3}}{z_2}(\frac{\partial Re}{\partial z_2}(.5e^{-Re} - (Re/2)e^{-Re} + .21\frac{Re^{-.5}}{F}(1 - e^{-Re} + .42\frac{Re^{1/2}}{F}e^{-Re})))]$$

$$\frac{\partial f_2}{\partial z_1} = \frac{\tilde{\mu}}{u_{l0}}\frac{\partial D}{\partial z_1} - z_2\frac{\partial \dot{M}}{\partial z_1}\frac{\tilde{\mu}}{u_{l0}z_1} + z_2\dot{M}\frac{\tilde{\mu}}{z_1^2 u_{l0}}$$

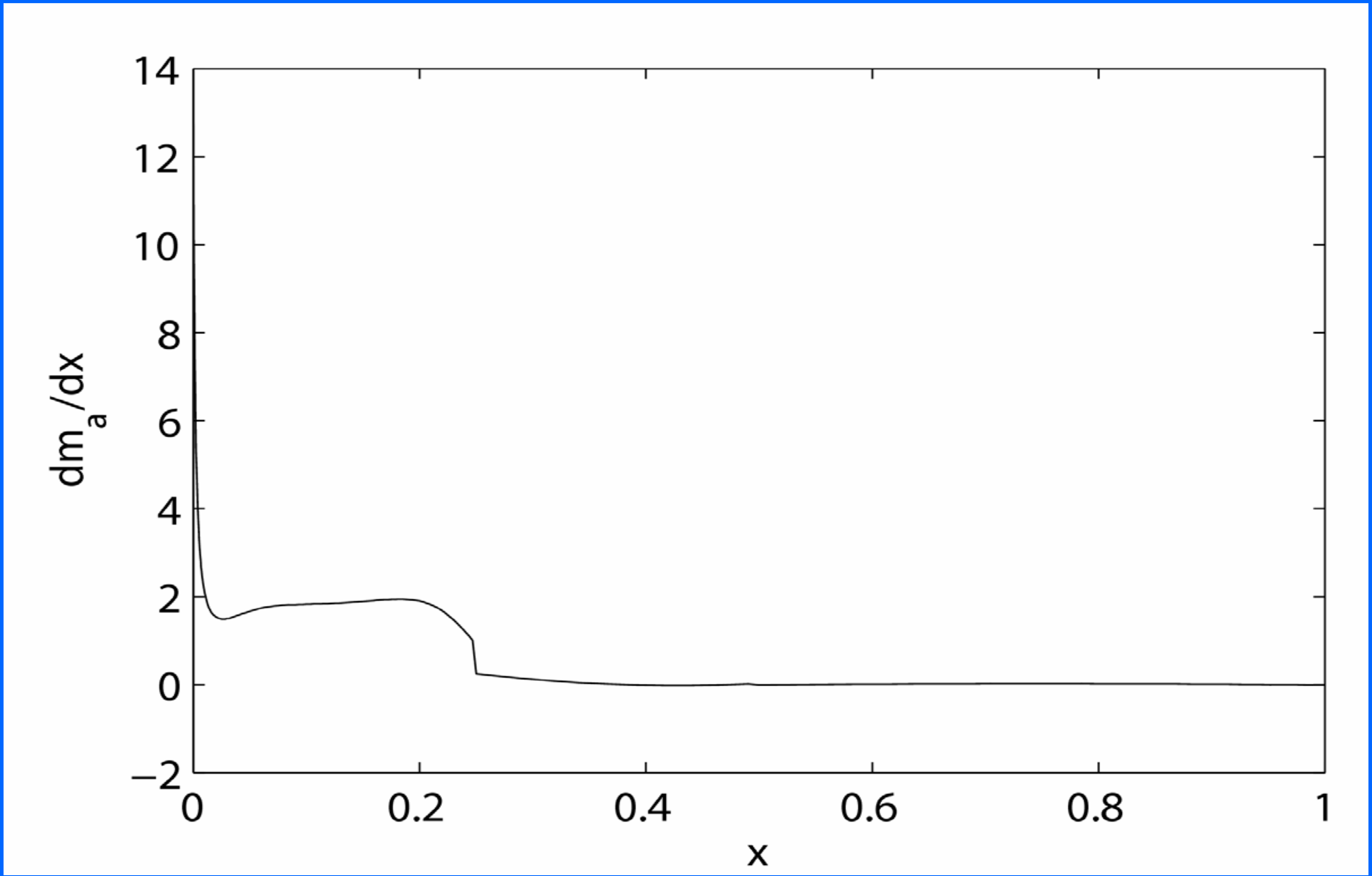
$$\frac{\partial f_2}{\partial z_2} = \frac{\tilde{\mu}}{u_{l0}}\frac{\partial D}{\partial z_2} - z_2\frac{\partial \dot{M}}{\partial z_2}\frac{\tilde{\mu}}{u_{l0}z_1} - \dot{M}\frac{\tilde{\mu}}{z_1 u_{l0}}$$

$$\frac{\partial L_{eff}}{\partial z_3} = \frac{-1}{Bz_1} - \frac{\partial B}{\partial z_3}\frac{(z_5 - (z_3/z_1))}{B^2}$$

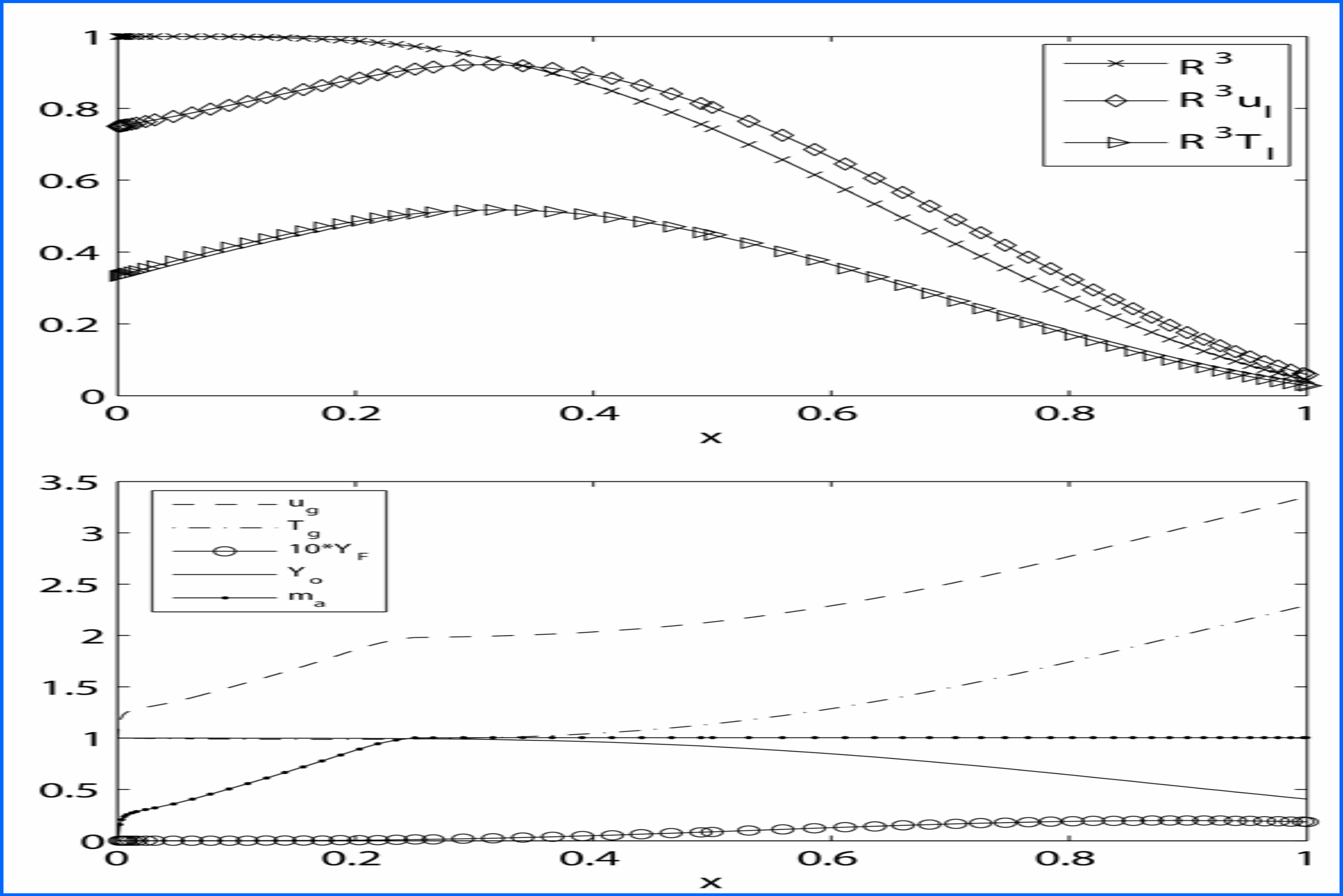
Parameters for one optimization

R¤ 0 = 60 *microns*, *L*¤ = 0:4 *m*;
u¤ *l0* = 30 *m/s*, *u*¤*g* 0 = 40 *m/s* ;
T¤ 0 = 900 *K*, *T*¤*l0* = 300 *K* ;
p = 10 *atm* .

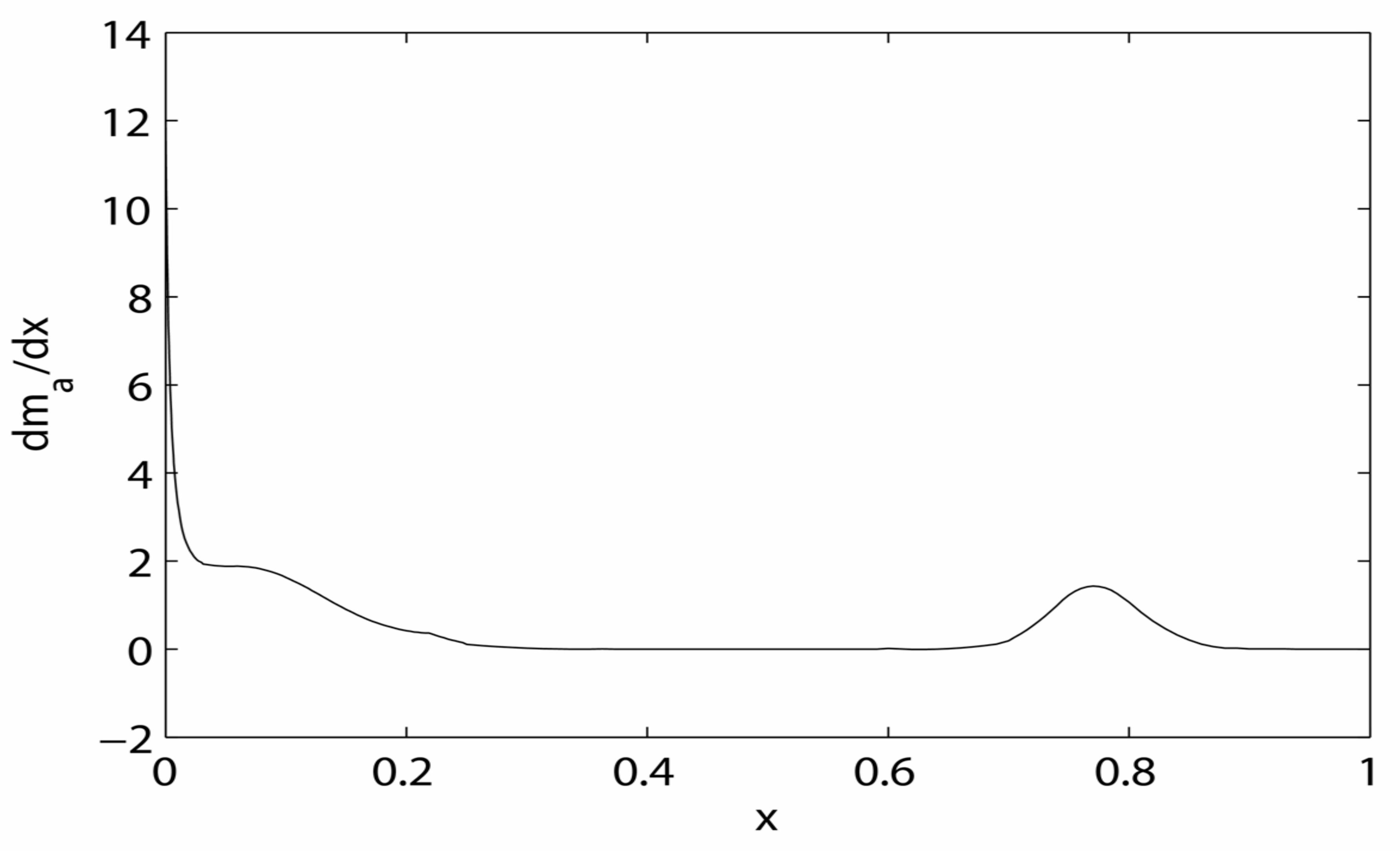
$$\frac{\partial Re}{\partial z_1} = \rho_g Re_0 \frac{1}{3z_1^{2/3}}|z_4 - \frac{z_2}{z_1}| + z_1^{1/3}\frac{z_2}{z_1^2}\frac{z_4 - \frac{z_2}{z_1}}{|z_4 - \frac{z_2}{z_1}|}$$



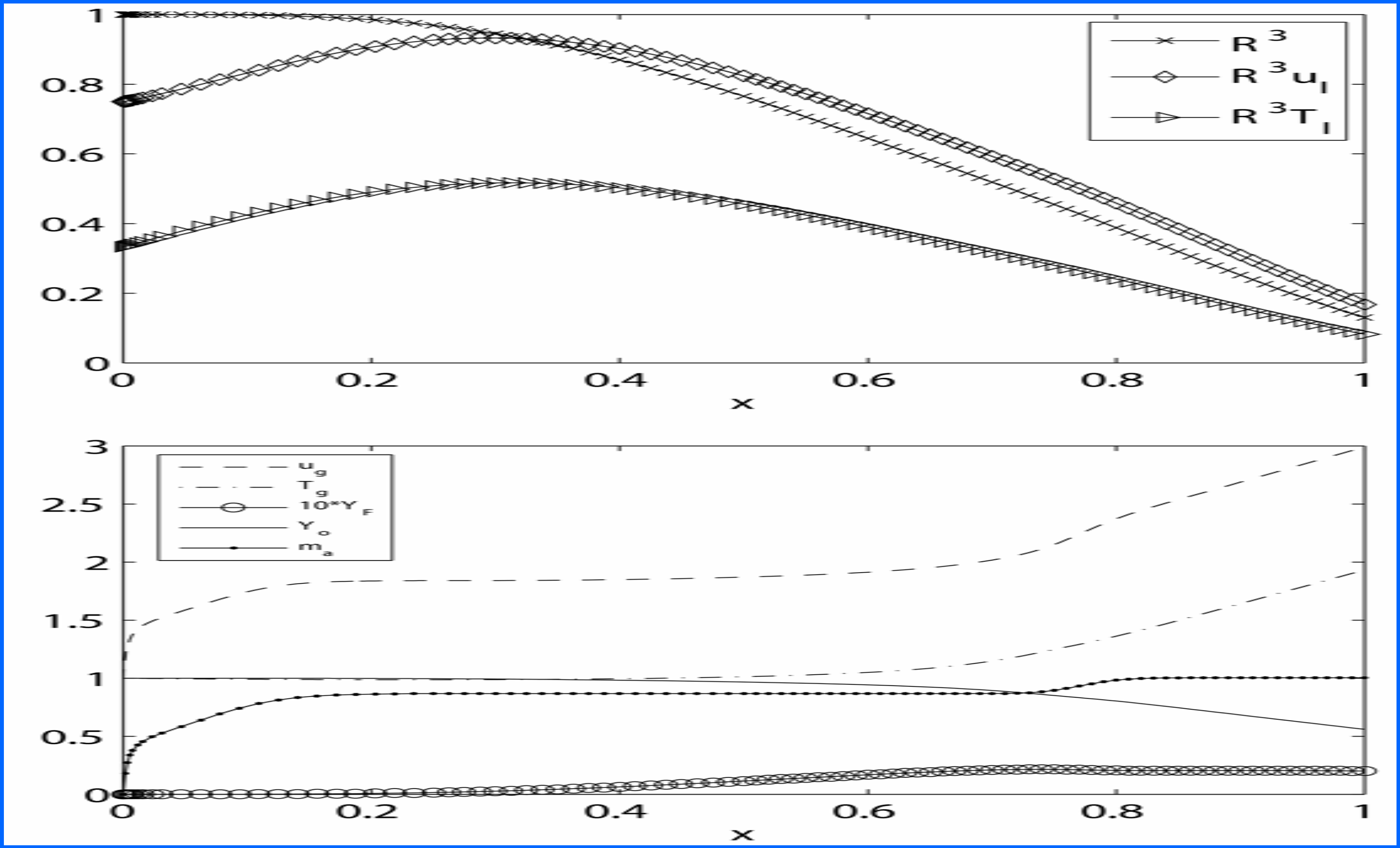
Optimal control for the Vaporization-Mixing model. Distribution of air-addition mass flux.



Optimal control for the Vaporization-Mixing model. Liquid-phase and gas-phase variables versus streamwise position.



Optimal control for the Vaporization-Mixing-Reaction model. Multimodal distribution of air-addition mass flux appears when more characteristic times are used.



Optimal control for the Vaporization-Mixing-Reaction model. Liquid-phase and gas-phase variables versus streamwise position.

Concluding Remarks

- **A framework for optimal control of combustors has been presented using the SLQ Algorithm.**
- **The optimization algorithm allows for placing constraints on exit values, interior-domain values, and integrals.**
- **Examples have been given for optimization of secondary-air addition to a continuous combustor using several appropriate spray combustion models.**
- **The challenge and the complexity of the resulting optimal control increases as the number of characteristic times increase.**

Thank you for your attention.

$$\dot{m}_d^* = \frac{|\dot{M}^*|}{n^*} = 4\pi\rho^* \tilde{D}^* R^* \log(1+B)\left[1 + \frac{Re}{2} e^{-Re} + \frac{0.6(2Re)^{0.5}(1-e^{-Re})}{F(B)}\right]$$

$$\begin{aligned} Re &= \rho|u-u_l|R \, Re_0 \\ &= \rho|u-u_l|R \, \frac{\rho_0^*|u_0^* - u_{l0}^*|R_0^*}{\mu_0^*} \end{aligned}$$

$$B = \frac{Y_{Fs}}{1 - Y_{Fs}}$$

$$F(B) = [1+B]^{0.7} \frac{\log(1+B)}{B}$$

$$L_{eff} = \frac{L^*_{eff}}{c^*_p T^*_0} \frac{T - T_l}{B}$$

$$Y_{Fs} = (1/p^*) e^{La^*/(\bar{R}^* T^*_b)} e^{-La/T_l}$$

$$\dot{M} = 4\pi c_1 \sigma_1 \sigma_2 \frac{z_1^{4/3}}{z_2} ln(1+B)h.$$

$$\sigma_1 = \frac{1}{1+e^{-\lambda_1(z_1-\epsilon_1)}}$$

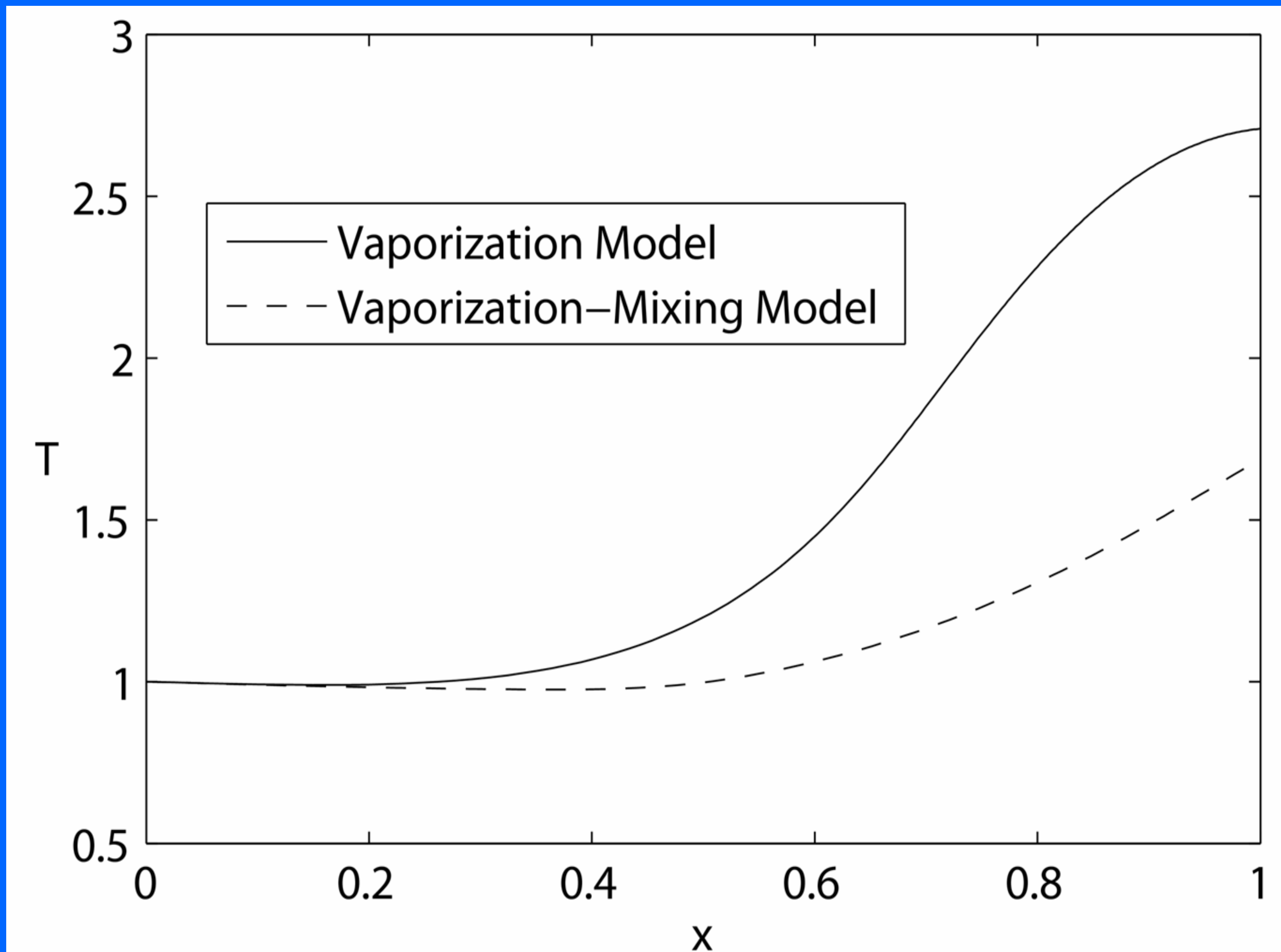
$$\sigma_2 = \frac{1}{1+e^{-\lambda_2(Y_O-\epsilon_2)}}.$$

$$D^* = n^* C_D \, \frac{1}{2} \, \rho^* (u^* - u_l^*) |u^* - u_l^*| \pi R^{*2}$$

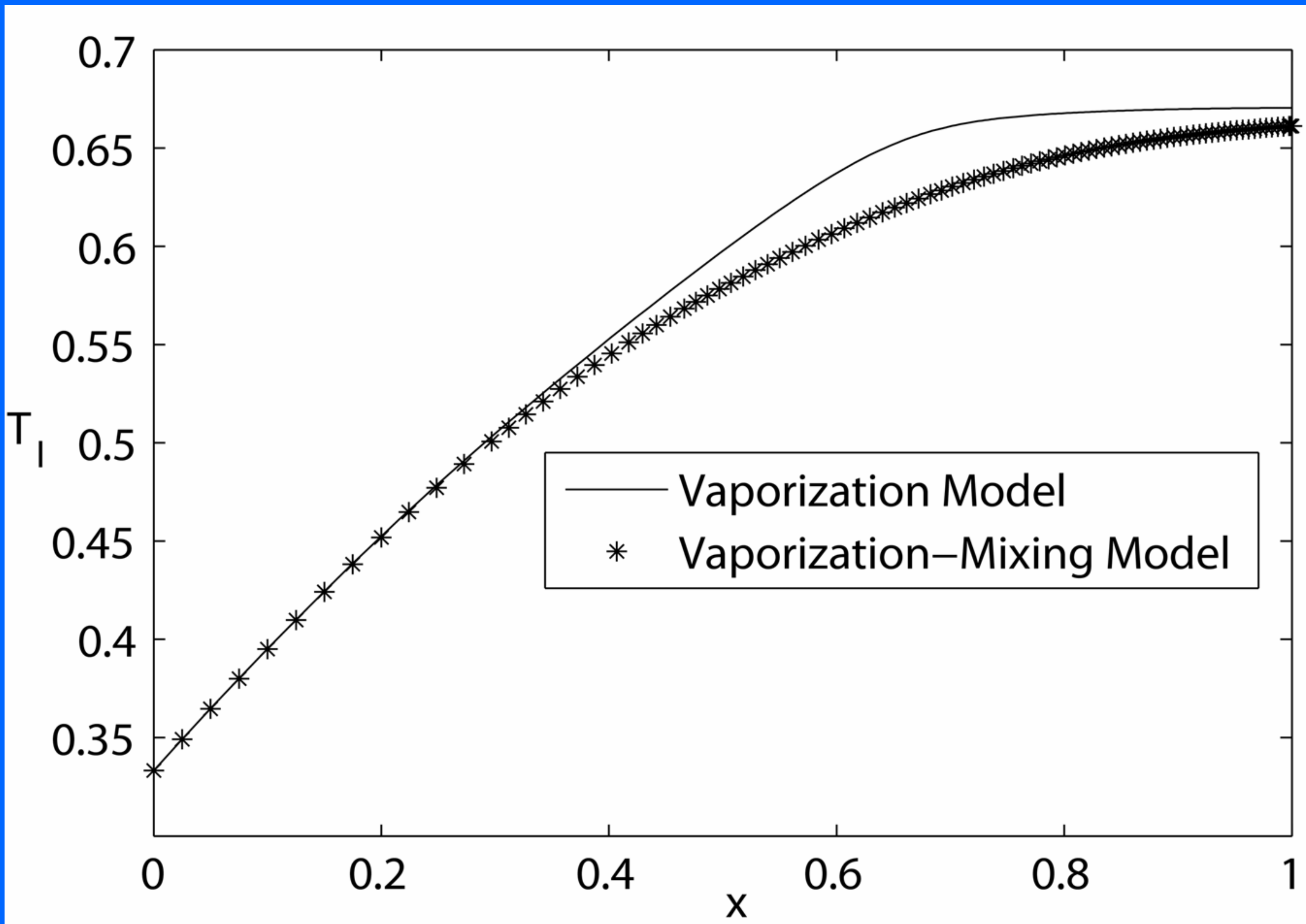
$$C_D = \frac{12}{Re\,(1+B)}$$

$$D = \frac{D^* L^*}{\rho_0^* u_0^{*2}} = \frac{6\pi c_1}{(1+B)} \, \frac{(u - u_l) R}{u_l}$$

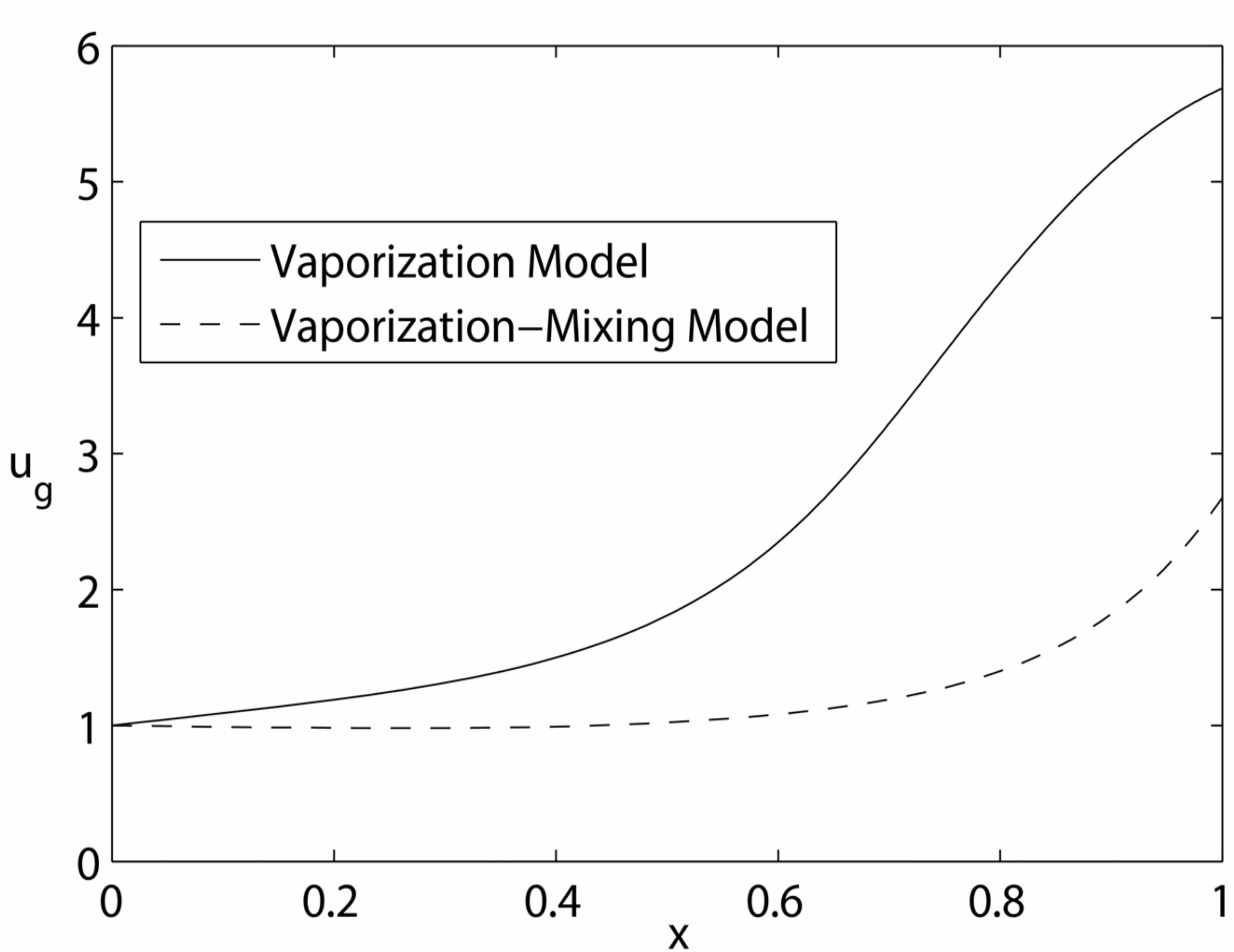
$$c_1 = \frac{3\rho_0^*}{4\pi\rho_l^*} \, \frac{\mu_0^* \dot{m}_f^*}{\dot{m}_0^{*2}} \, \frac{L^* A^*}{R_0^{*2}}$$



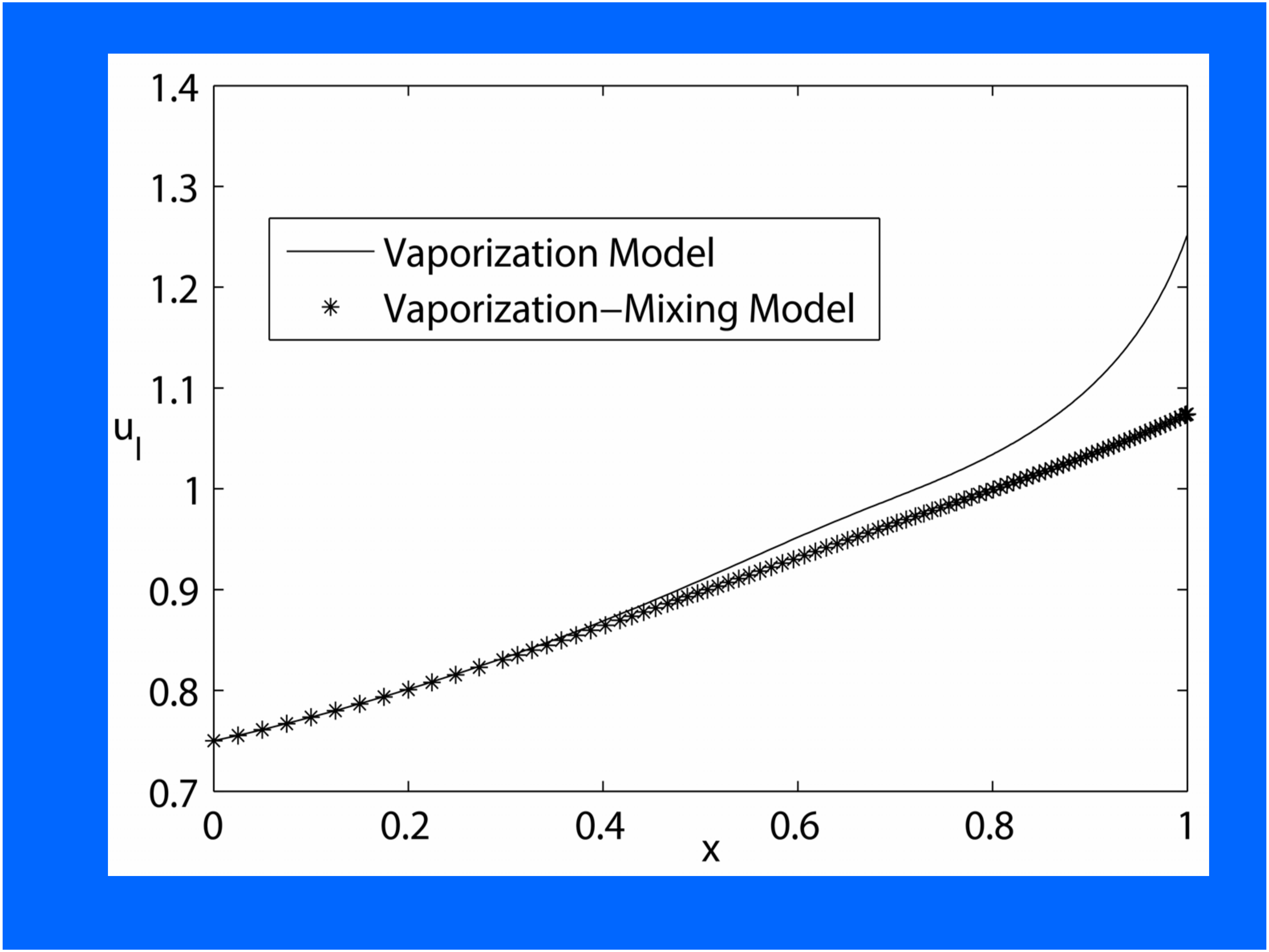
Vaporization Model
Vaporization−Mixing Model
T
x
3
2.5
2
1.5
1
0.5
0
0.2
0.4
0.6
0.8
1



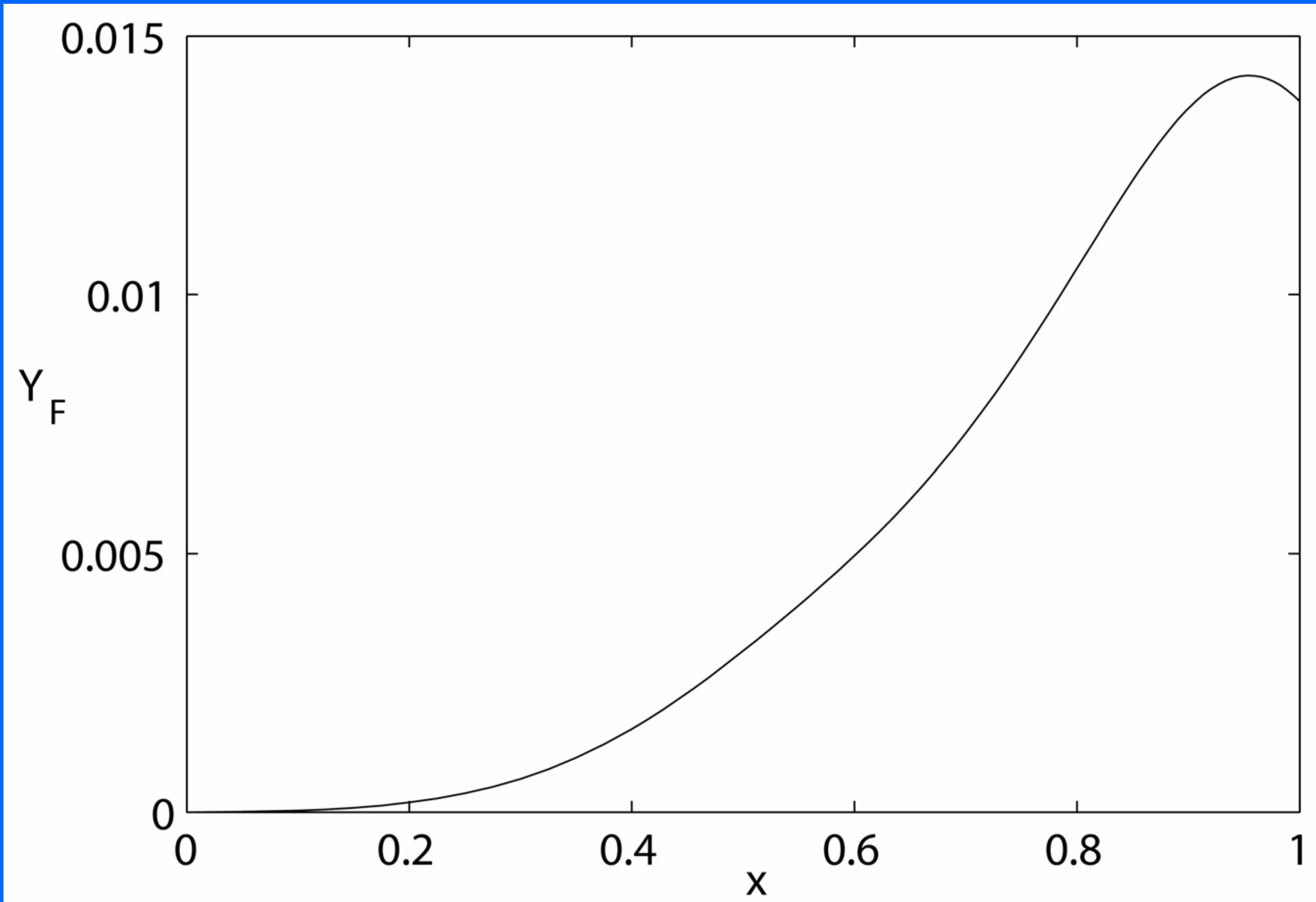
0.7
0.65
0.6
0.55
0.5
0.45
0.4
0.35
T l
0
0.2
0.4
0.6
0.8
1
x
Vaporization Model
Vaporization–Mixing Model

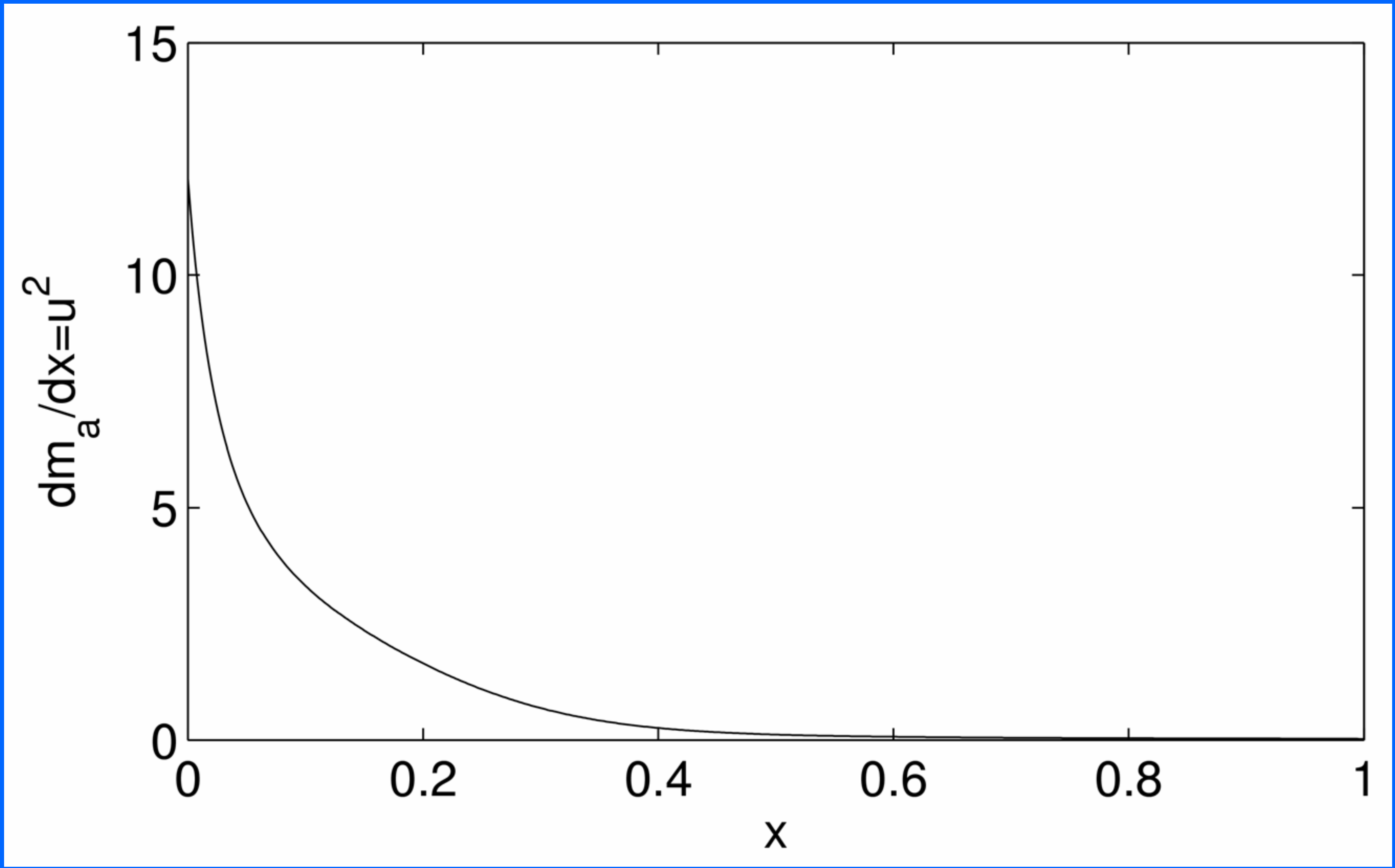


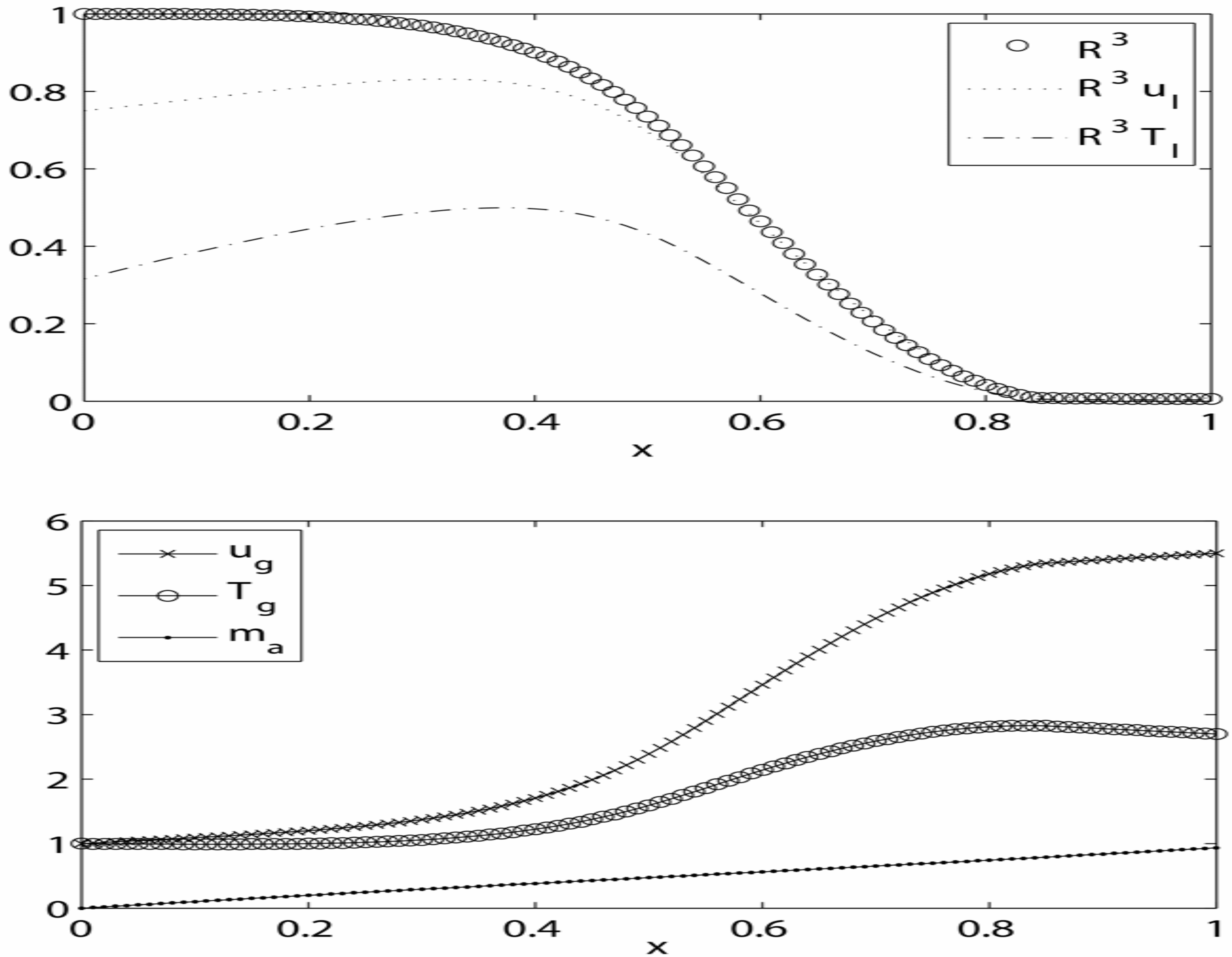
Vaporization Model
Vaporization−Mixing Model
u_g
x
0
1
2
3
4
5
6
0
0.2
0.4
0.6
0.8
1



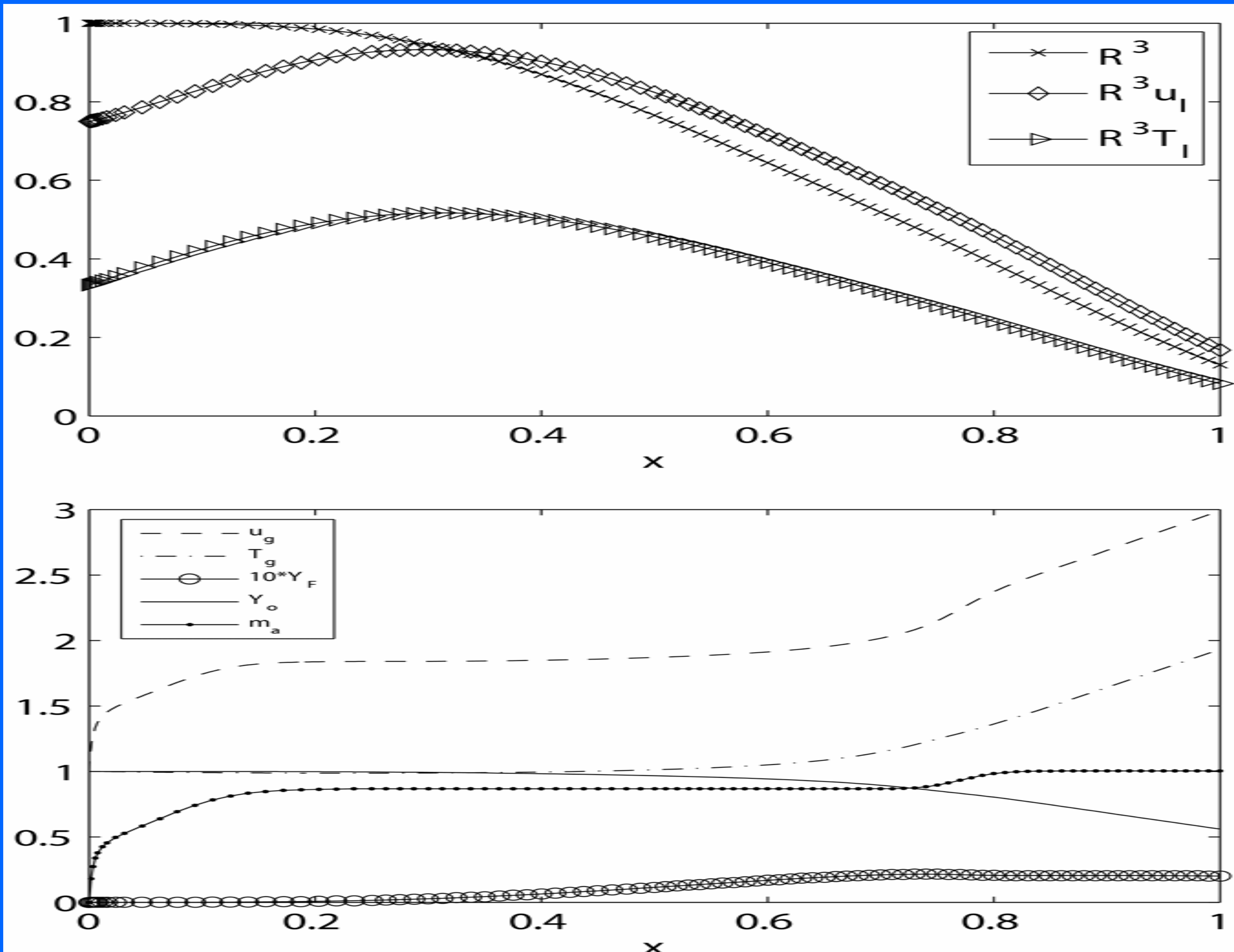
1.4
1.3
1.2
1.1
1
0.9
0.8
0.7
u_l
0
0.2
0.4
0.6
0.8
1
x
Vaporization Model
Vaporization−Mixing Model


0.015
0.01
0.005
0
Y_F
0
0.2
0.4
0.6
0.8
1
x


15
10
5
0
$dm_a/dx=u^2$
0
0.2
0.4
0.6
0.8
1
x



R^3
R^3 u_l
R^3 T_l
0
0.2
0.4
0.6
0.8
1
x
u_g
T_g
m_a
0
1
2
3
4
5
6
0
0.2
0.4
0.6
0.8
1
x



R 3
R 3u l
R 3T l
0
0.2
0.4
0.6
0.8
1
x
u g
T g
10*Y F
Y o
m a
0.5
1.5
2
2.5
3

$$\lambda(n) = \lambda(n+1)\mathbf{F}_z(\mathbf{z}(n), U(n)) + L_z(\mathbf{z}(n), U(n))$$

$$\lambda(N) = \Phi_z(\mathbf{z}(n))$$

$$H_u(\lambda(n+1), \mathbf{z}(n), U(n)) = 0$$

$$H(\lambda, \mathbf{z}, U) = \lambda^T \mathbf{F}(\mathbf{z}, U) + L(\mathbf{z}, u)$$