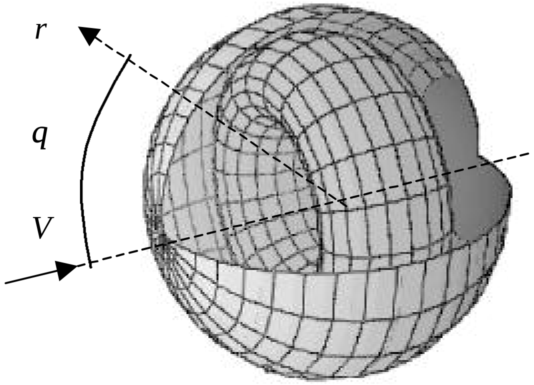
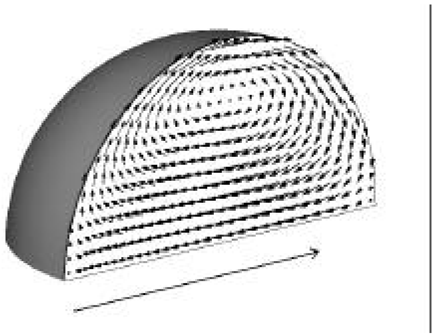
New Drop Evaporation Models for FIRE Spray Module

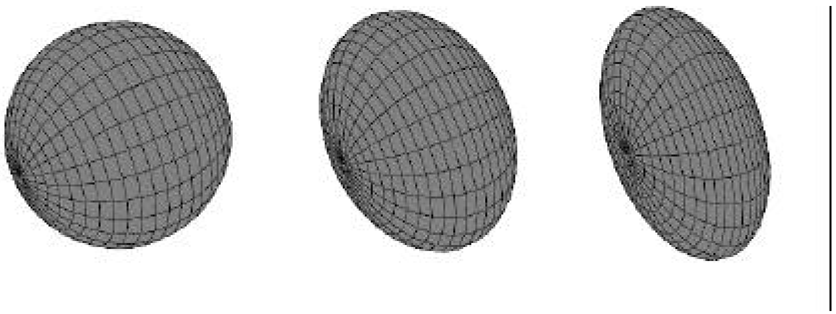
Frolov Sergey
Semenov Institute of Chemical Physics
Moscow, Russia
smfrol@chph.ras.ru

Objective I

Develop and implement a drop evaporation model which incorporates the effects of internal liquid circulation and drop deformation in the gaseous flow

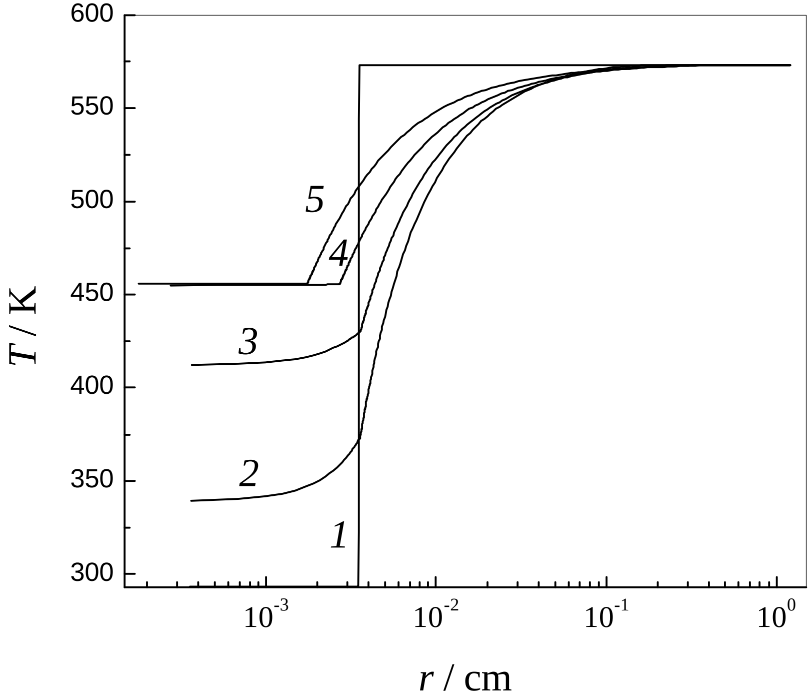






Objective II

Develop and implement a drop evaporation model which incorporates the effects of transient heat and mass transfer between drop and gas



~40% of drop lifetime

$C_{14}H_{30}$, 70 μm

Detailed model

$$\frac{dm_d}{dt} = 4p\, r_d^2\, r_{l\,s} u_s \qquad c_l\, r_l \frac{\partial T_l}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(l_l r^2 \frac{\partial T_l}{\partial r} \right)$$

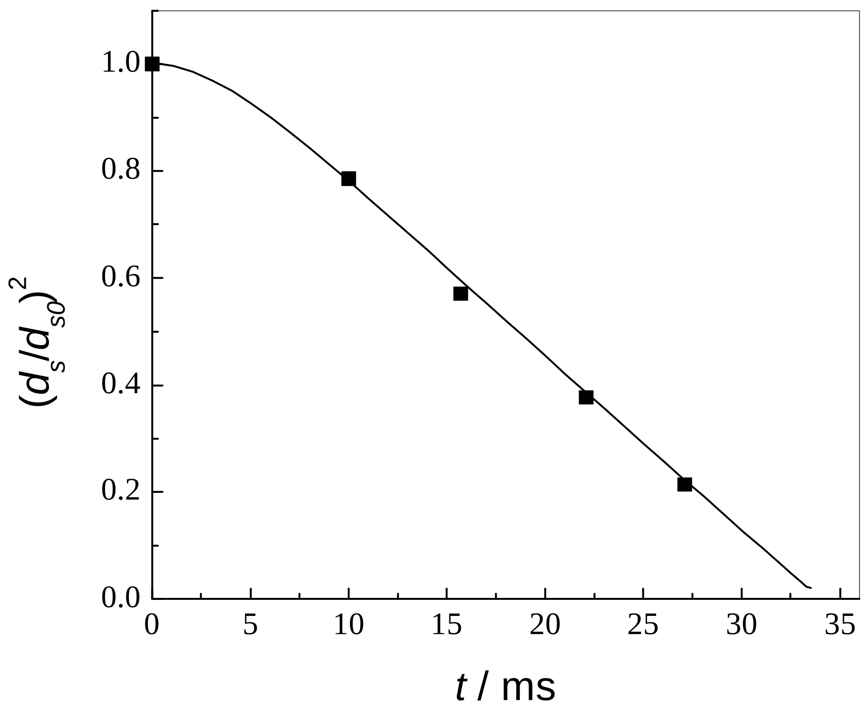
$$\frac{\partial r_g}{\partial t} + \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 r_g u_g\right) = 0$$

$$r_g \frac{\partial Y_i}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r_g r^2 Y_i V_i\right) - r_g u_g \frac{\partial Y_g}{\partial r}$$

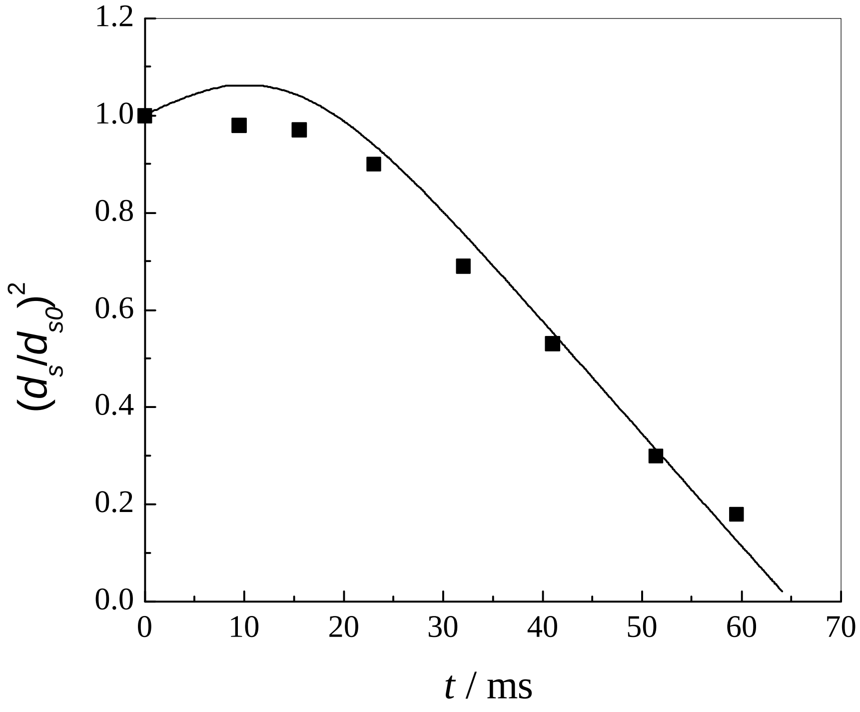
$$\frac{\partial X_i}{\partial r} = \sum_{j=1}^{N}\left(\frac{X_i X_j}{D_{ij}} \right)\left(V_j - V_i\right)$$

$$c_{pg}\, r_g \frac{\partial T_g}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(l_g r^2 \frac{\partial T_g}{\partial r} \right) - c_{pg}\, r_g u_g \frac{\partial T_g}{\partial r}$$

Detailed model validation



C_7H_{16}, 70 µm



$C_{14}H_{30}$, 70 µm

Exp.: Massoli (1993)

Model I: Phenomenology

Energy balance equation for drop

$$c_d m_d \frac{dT_d}{dt} = \dot{Q}_{i-}$$

$$\dot{Q}_{i-} = f(t, T_i, T_d, U_i, \ldots) \rightarrow c_d m_d \frac{dT_d}{dt} = \dot{Q} + H \frac{dm_d}{dt}$$

$$T_d = T_i = T_{wb} \rightarrow \dot{Q} = -H \frac{dm_d}{dt}$$

$$\dot{Q} = S_d q \qquad q = h(T_g - T_i) \qquad h = \frac{\mathrm{Nu}}{d} l_g \frac{\ln(1+B)}{B}$$

Equation of drop motion

$$m_d \frac{dV}{dt} = \frac{1}{2} r_g \underline{A} C_D V \left| V \right|$$

$$\underline{C_D} = \frac{C_{Ds}}{(1 + B)}$$

Equation of drop mass balance

$$\frac{dm_d}{dt} = -\underline{S_d}\, j$$

$$j = 2 \frac{r_g D}{d} \ln(1 + B)$$

Effects

(1) effect of internal liquid circulation on the duration of the transient drop-heating period

(2) temporal variation of the drop cross-section area *A* due to drop deformation

(3) increase in the drop surface area S_d due to drop deformation

(4) temporal variation of the drop drag coefficient due to drop deviation from the spherical shape

(5) temporal variation of the drop drag coefficient due to vaporization and

(6) temporal variation of the heat transfer coefficient due to drop deviation from the spherical shape.

Wet-bulb temperature

$$t_l = \underline{t_h} + \Delta t_{qs}$$

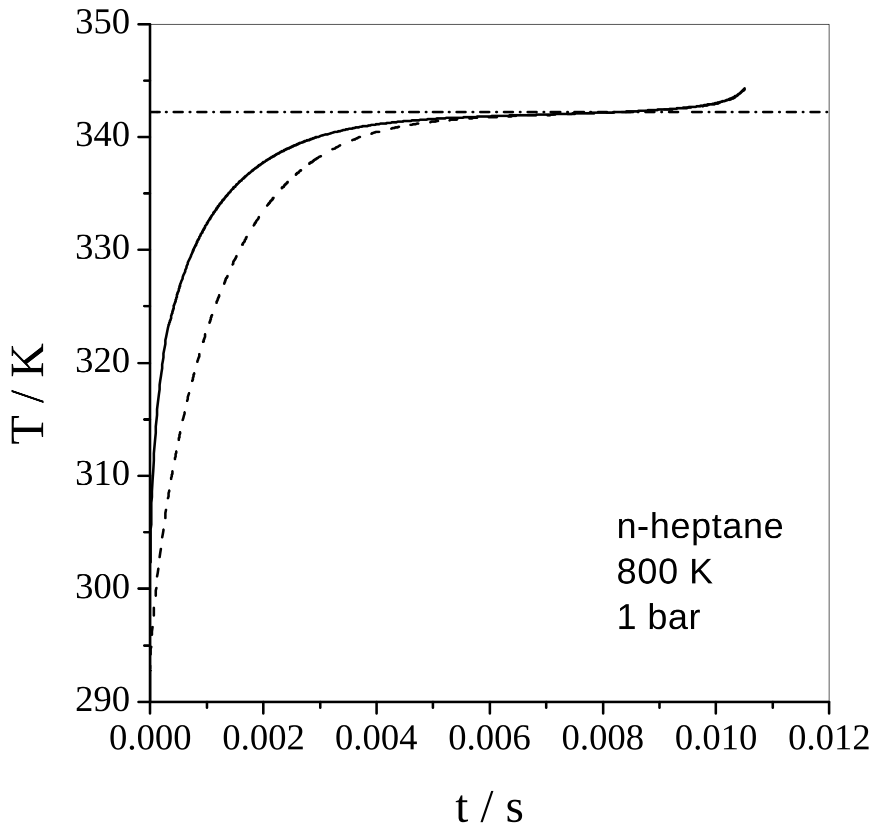
At t > t$_h$ $\dot{Q} = -H \frac{dm_d}{dt}$

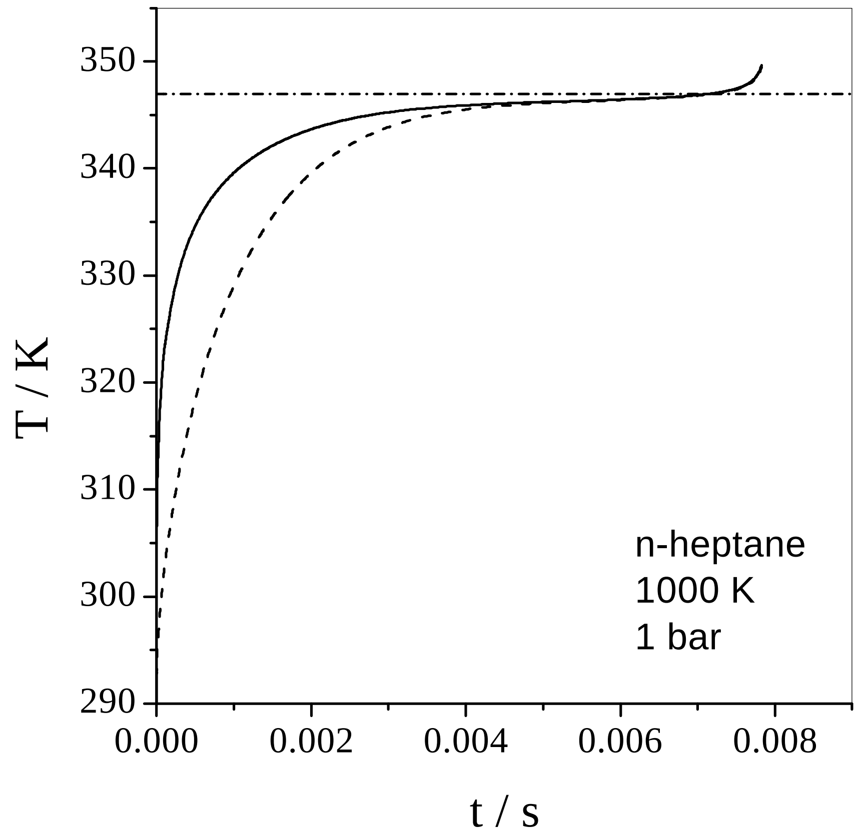
For heavy hydrocarbons t$_l$ ~ t$_h$

$$\mathrm{Nu}\, l_g (T_g - T_i) = 2\, r_g DH \frac{Y_{vi} - Y_{v\infty}}{1 - Y_{vi}}$$

Wet-bulb temperature: Validation

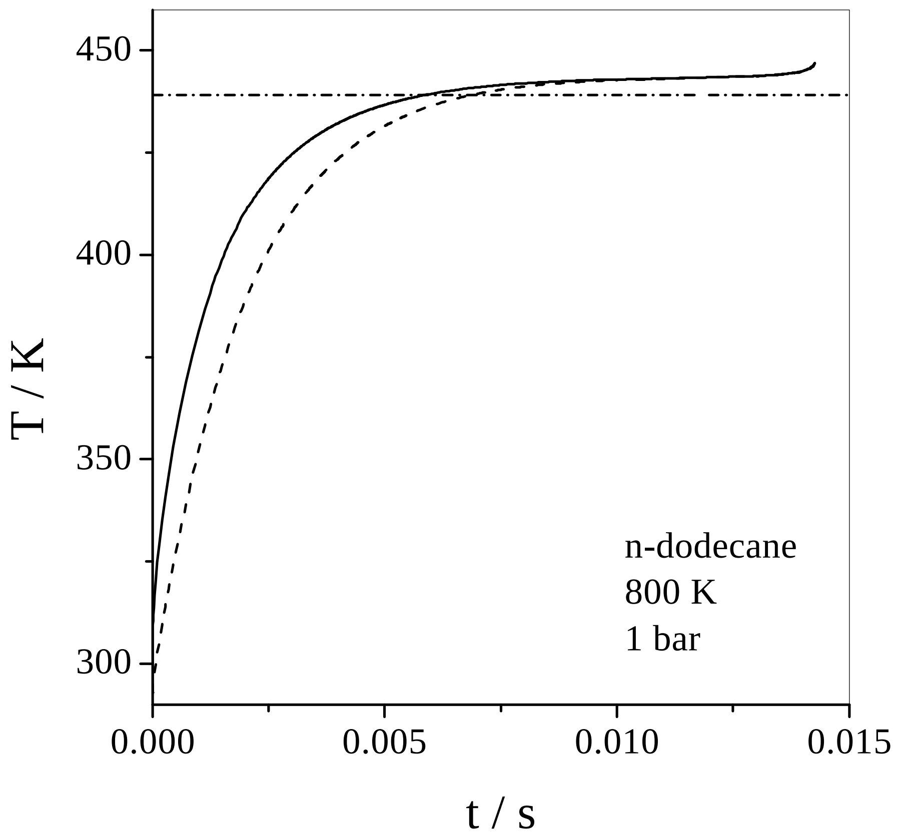
n-heptane, 1 bar

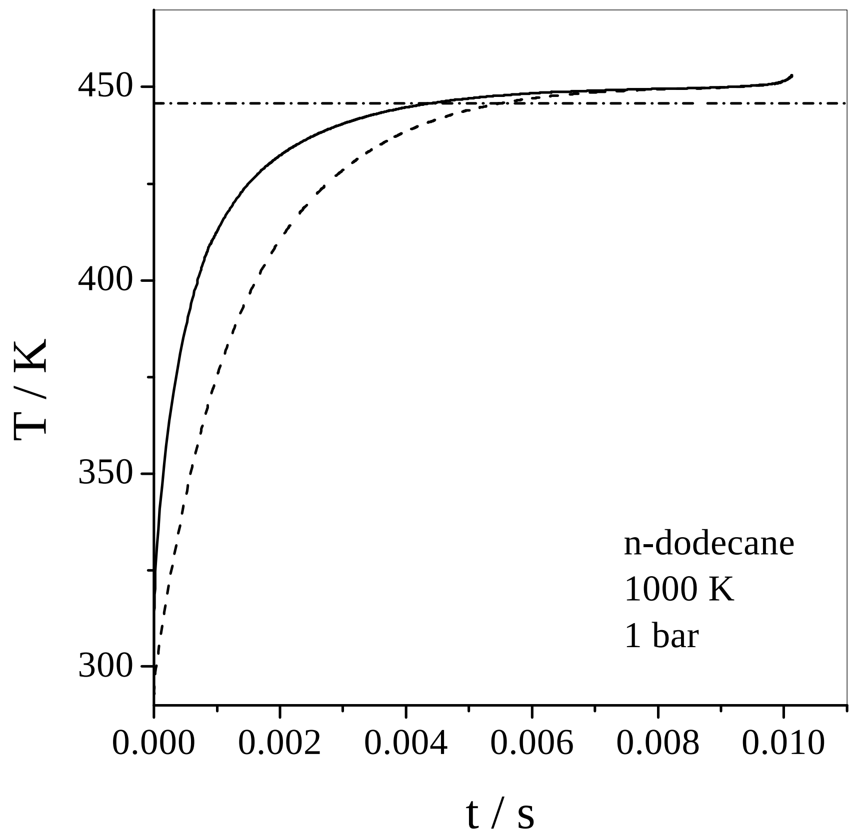




Wet-bulb temperature: Validation

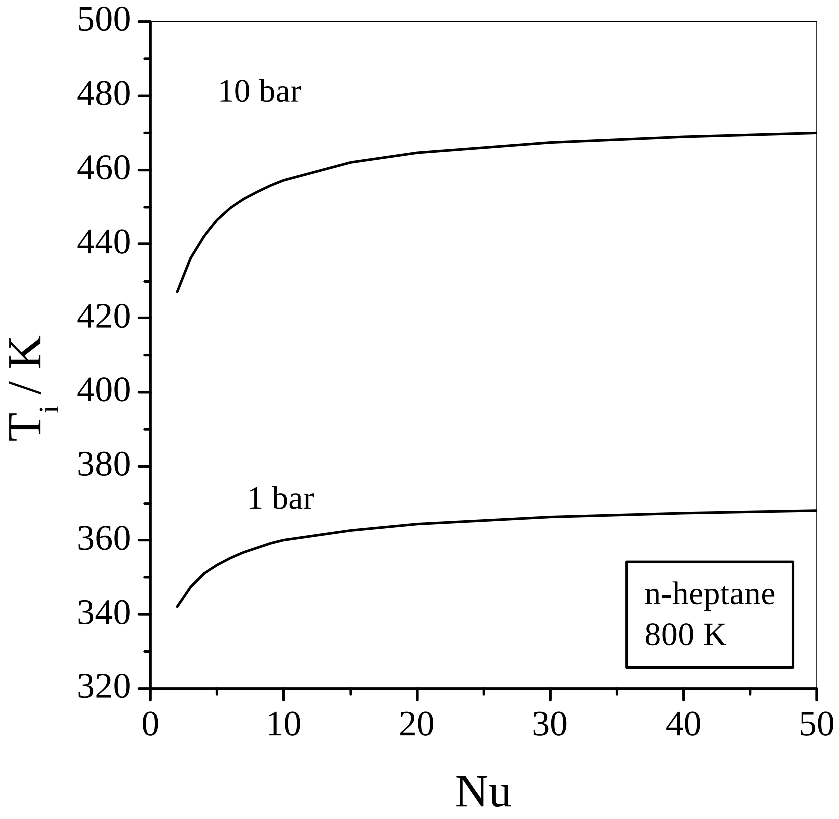
n-dodecane, 1 bar

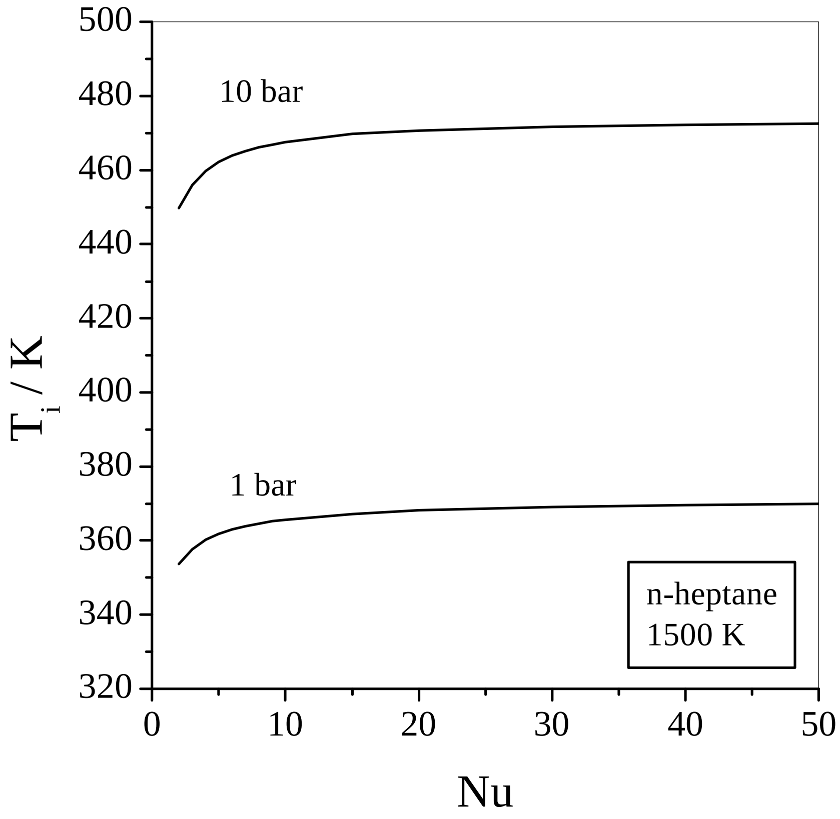




Pressure and Re effects

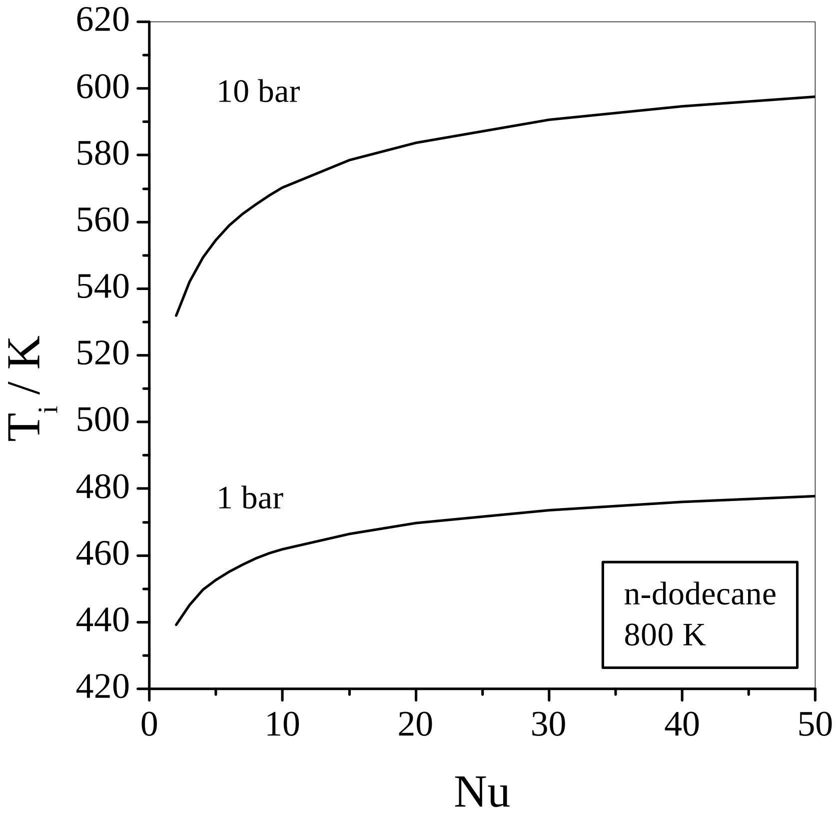
n-heptane

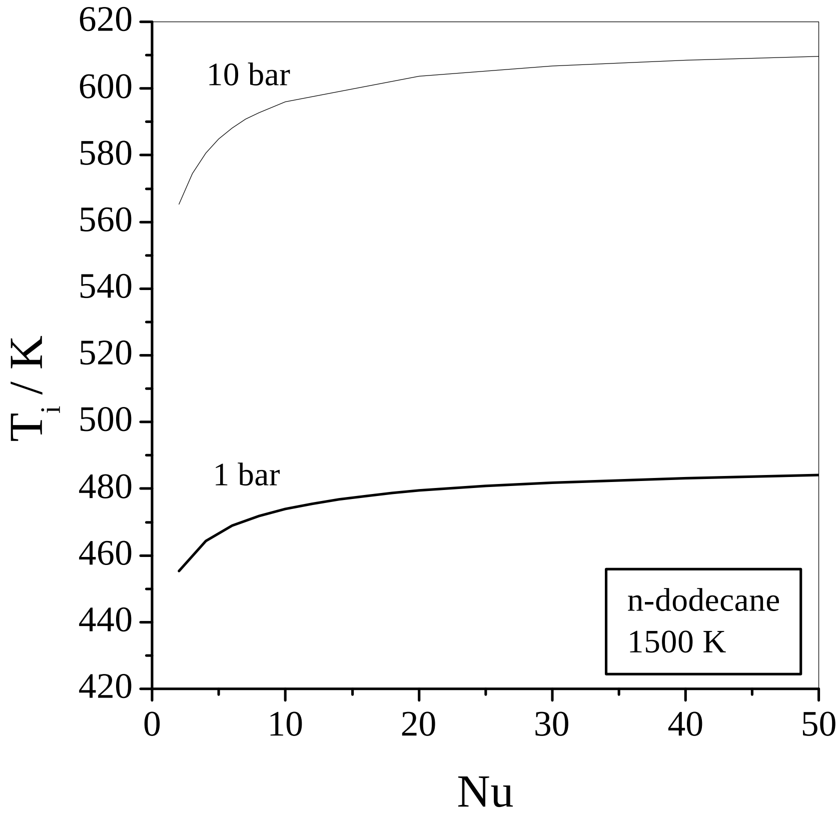




Pressure and Re effects

n-dodecane





Main assumptions

- Heating of the evaporating drop interior occurs at constant surface temperature
- To estimate the surface temperature one can use $Nu = Nu_{qs} = 2$
- The problem is reduced to internal problem of drop heating

Spherical drop heating with internal circulation

$$U_q = -U_i\left(1 - 2r^2 / R^2\right)\sin q$$

$$U_r = U_i\left(1 - r^2 / R^2\right)\cos q$$

$$U(X,Y) = U_i \exp\left[-Y / \left(b\sqrt{X}\right)\right]$$

$$U_i = aV$$

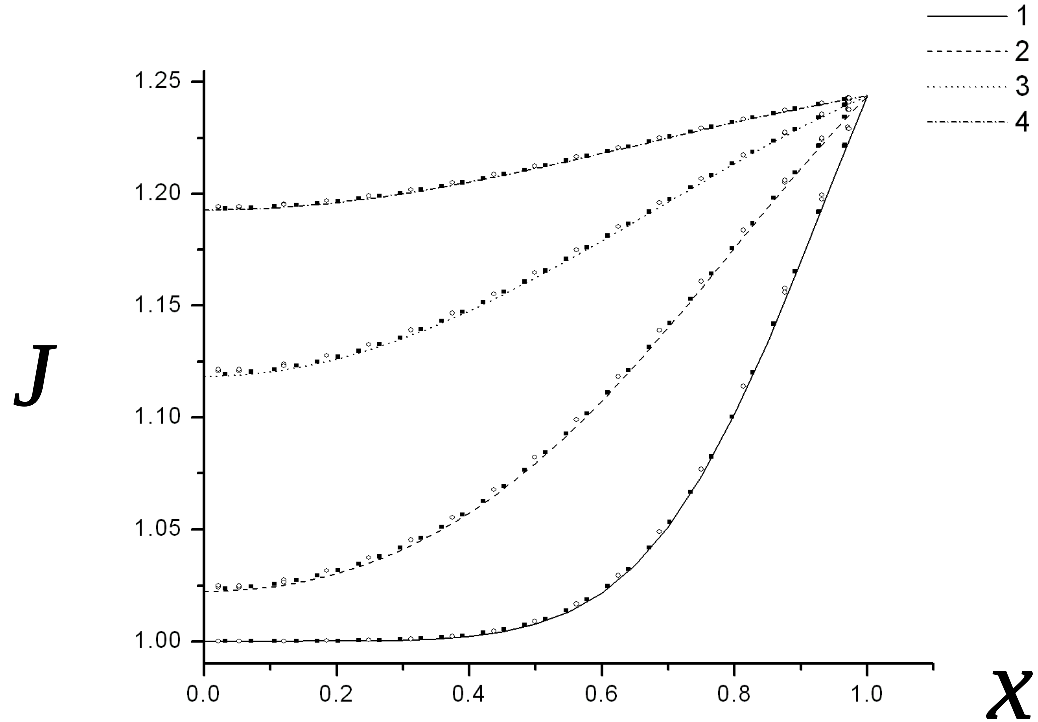
$$a = \left[r_g m_g / (r_d m_d)\right]^{1/3}, \;\; b = \left[4m_d / (a r_d V)\right]^{1/2}$$

$$\frac{\partial T}{\partial t} + U_r \frac{\partial T}{\partial r} + \frac{U_q}{r}\frac{\partial T}{\partial q} = a_T\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial T}{\partial r}\right) + \frac{1}{r^2 \sin q}\frac{\partial}{\partial q}\left(\sin q \frac{\partial T}{\partial q}\right)\right]$$

Validation: no circulation

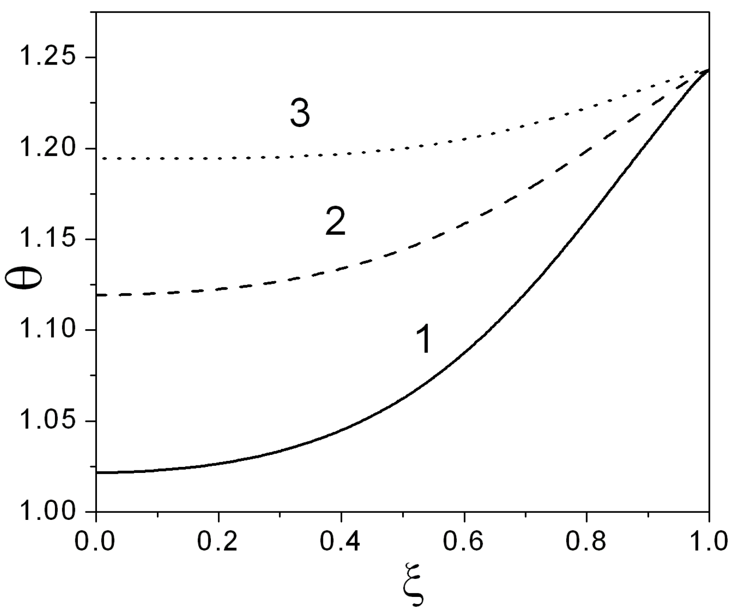
$$J(x,t) = J_i + (J_i - 1)\frac{2}{\pi x}\sum_{m=1}^{\infty}\frac{(-1)^m}{m}\sin(\pi m x)\exp(-\pi m w t)$$

$$h = \frac{J_{\min} - 1}{J_i - 1}$$

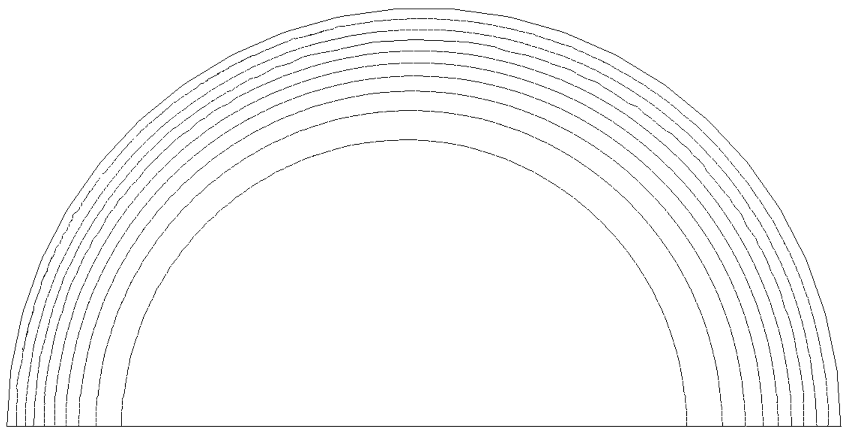


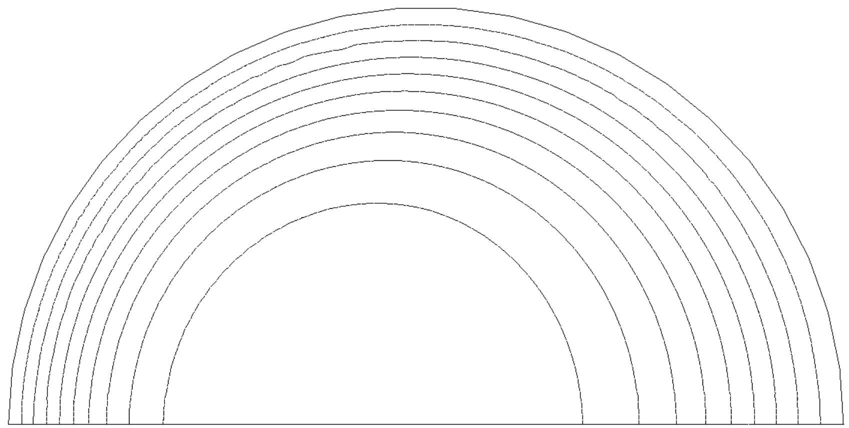
Heat transfer modes for a spherical drop

Conductive mode



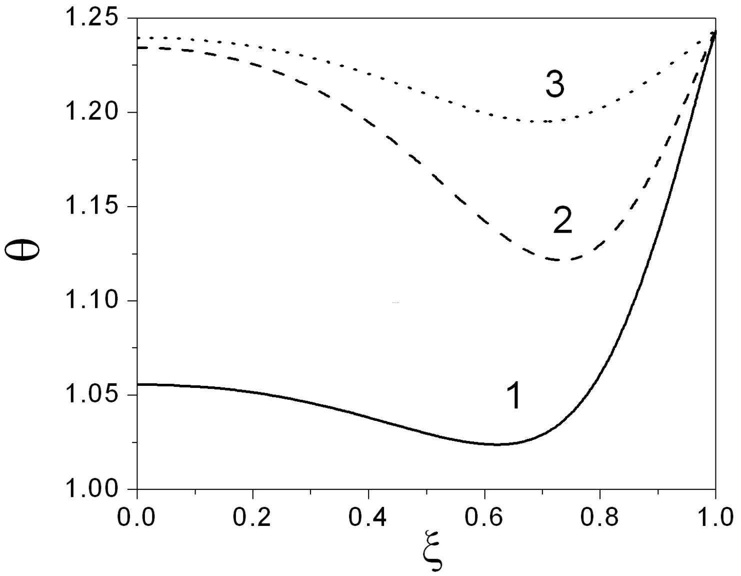
Rel = 1.7



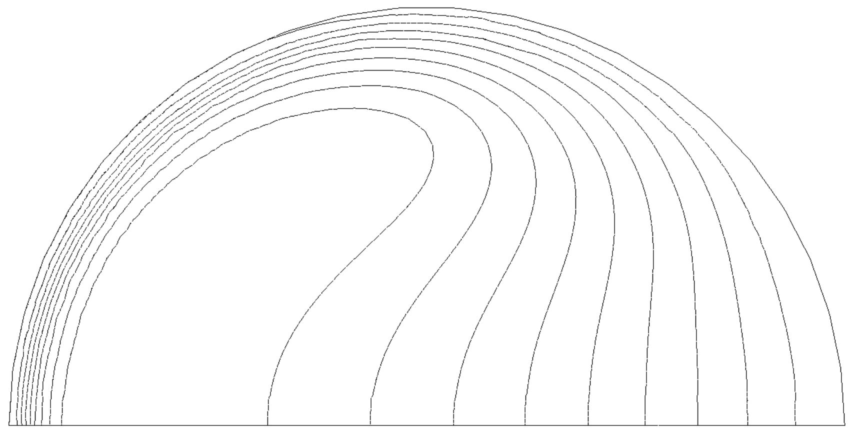
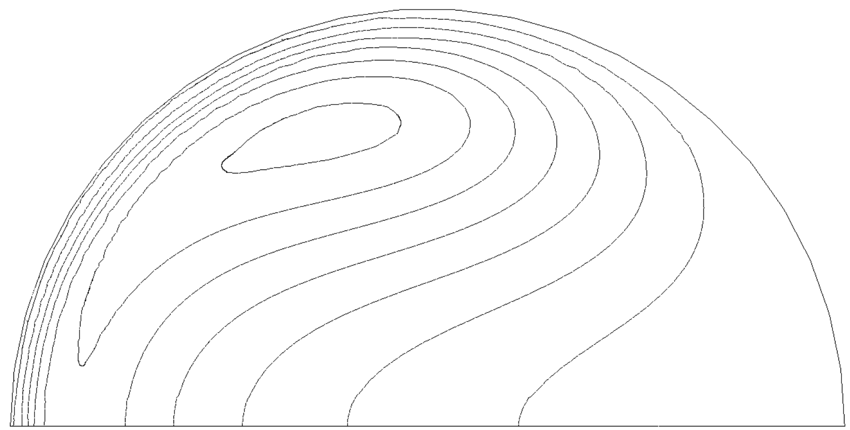


Heat transfer modes for a spherical drop

Transient mode

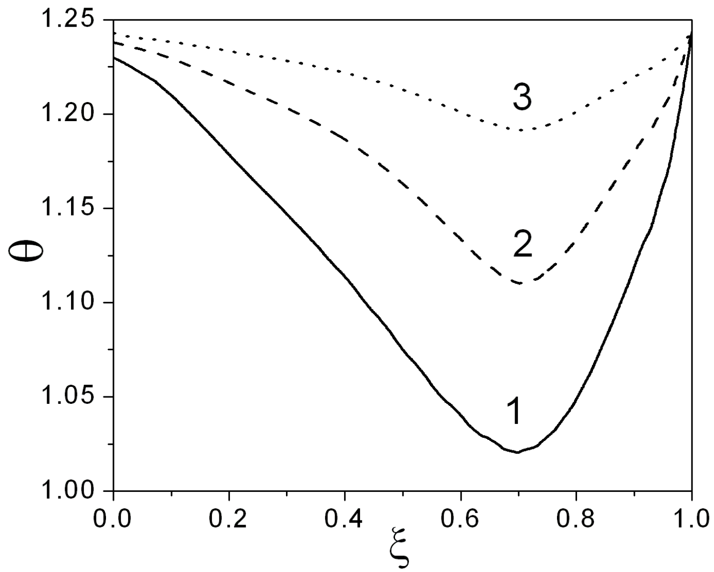


Reₗ = 17

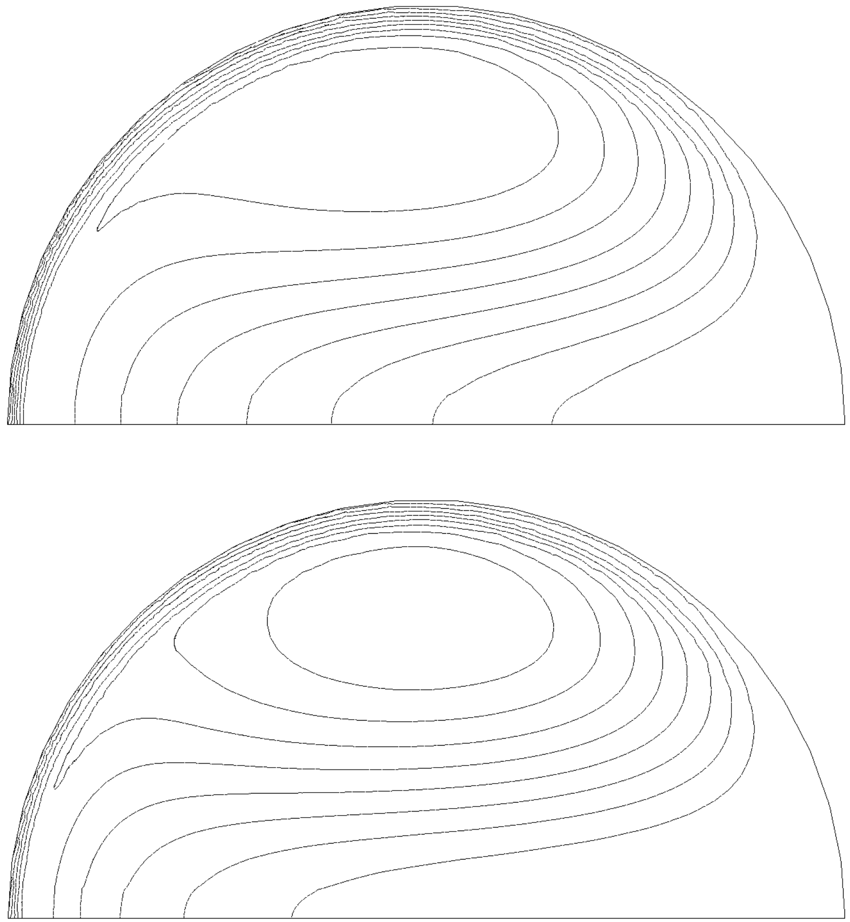



Heat transfer modes for a spherical drop

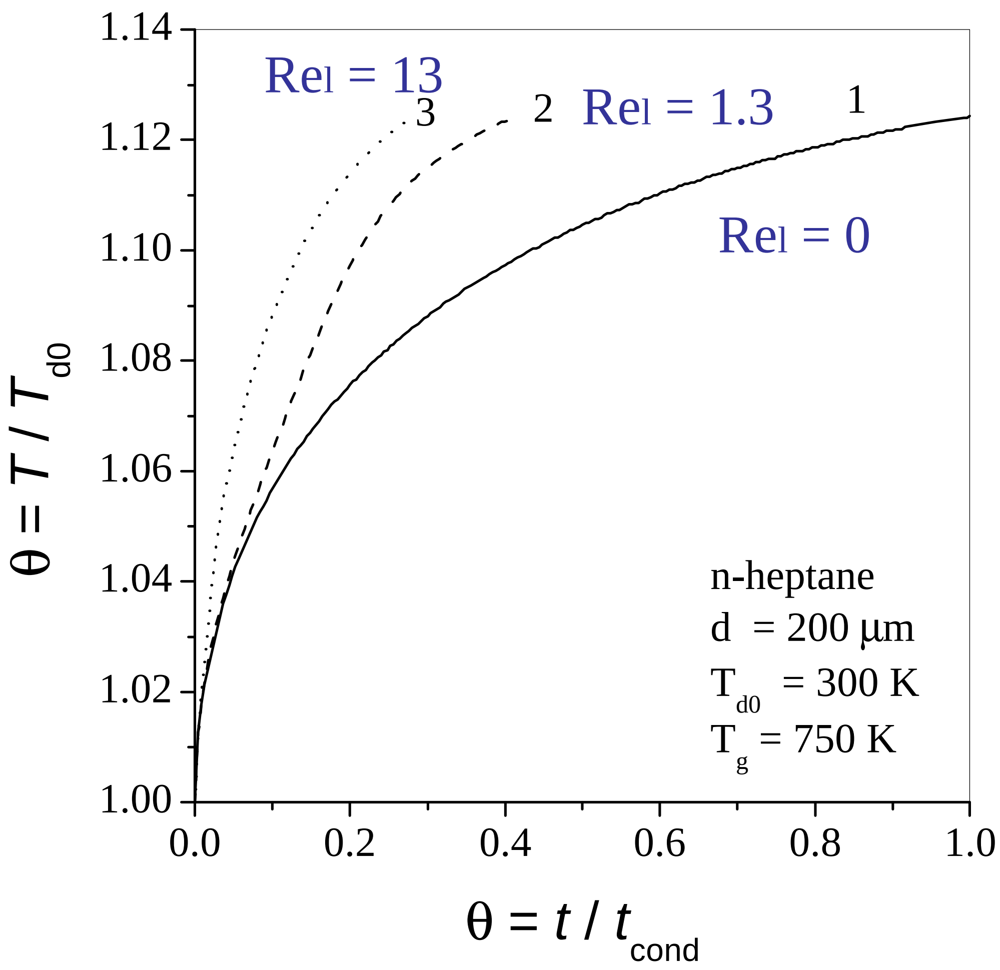
Convective mode



$Re_l = 170$

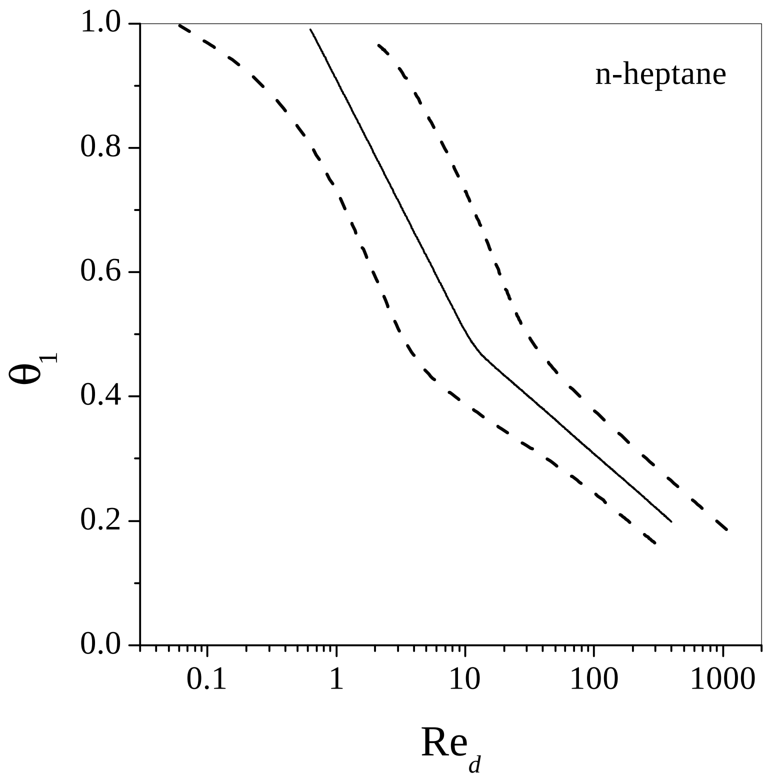


Mean temperature history

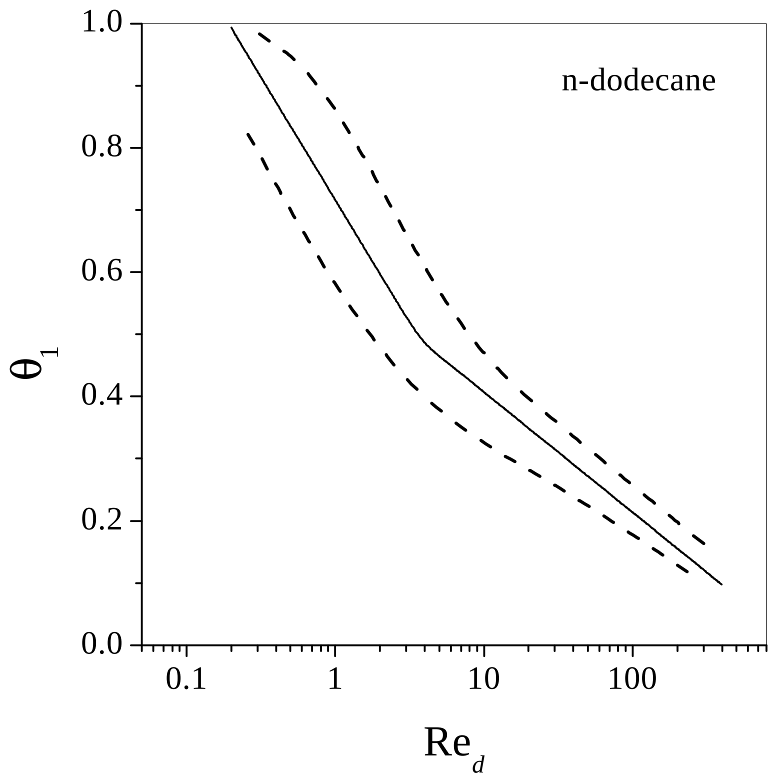


Heat flux correction factors for spherical drops

n-heptane



n-dodecane



Heat flux correction factors for spherical drops: Correlations

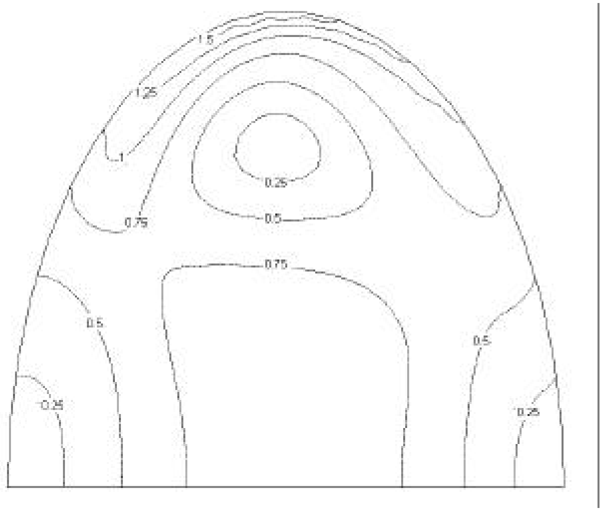
$$Q_{i-} = q_1^{-1} Q_{i-}^{o}$$

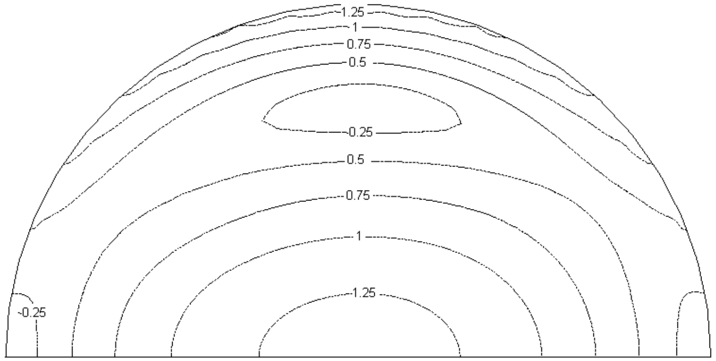
$$q_1 = 1 \text{ at } \mathrm{Re_d} \le \mathrm{Re}_d^{*}$$

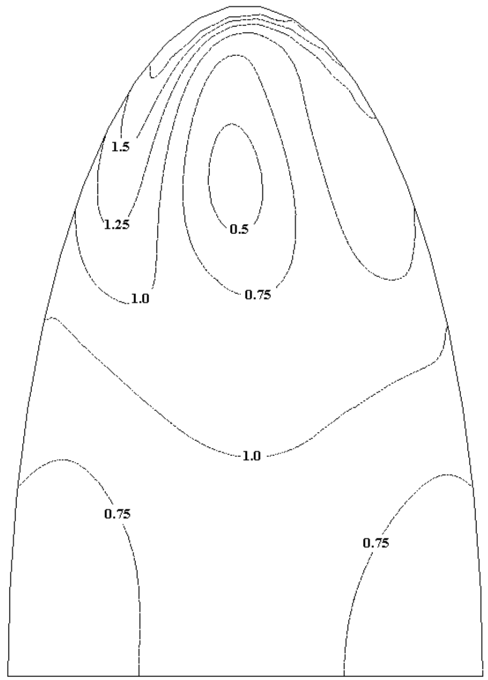
$$q_1 = C_1 \log(\mathrm{Re}_d) + C_2 \text{ at } \mathrm{Re}_d^{*} < \mathrm{Re}_d < \mathrm{Re}_d^{**}$$

$$q_1 = C_3 \log(\mathrm{Re}_d) + C_4 \text{ at } \mathrm{Re}_d > \mathrm{Re}_d^{**}$$

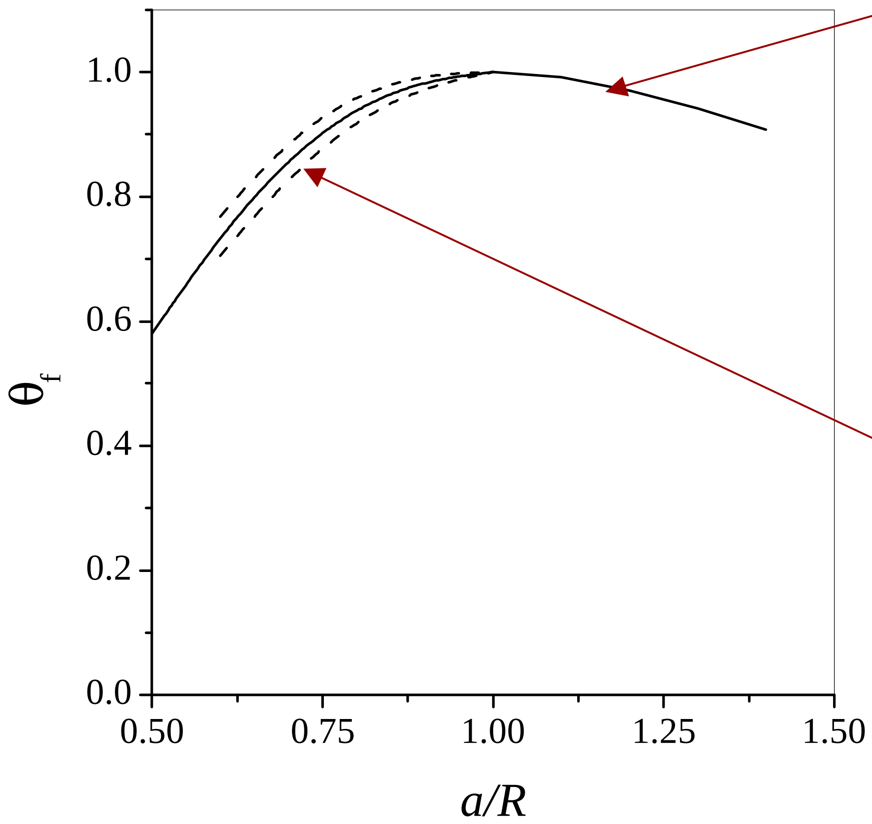
Deformed drop: Velocity distributions







Heat flux correction factors for deformed drops



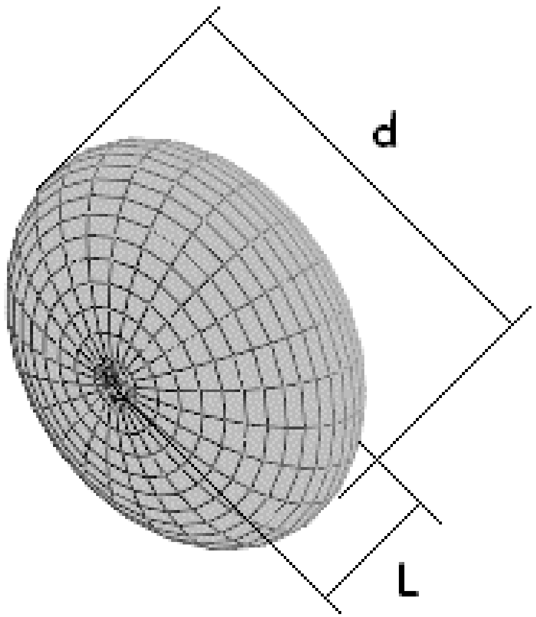
$$q_f = 0.65 + 0.77\left(\frac{a}{R}\right) - 0.42\left(\frac{a}{R}\right)^2$$

$$q_f = -0.78 + 3.67\frac{a}{R} - 1.89\left(\frac{a}{R}\right)^2$$

$$Q_{i-} = q_f^{-1} Q_{i-}^{o}$$

Drop deformation

$$\ddot{y} = \frac{C_F}{C_b}\frac{r_g}{r_d}\frac{V^2}{R^2} - \frac{C_k s}{r_d R^3} y - \frac{C_d m_d}{r_d R^2}\dot{y}$$



$$y = \frac{x}{C_b R}$$

$$Q_{i-} = q_1^{-1} q_f^{-1} Q_{i-}^{o}$$

Increase in the drop surface area

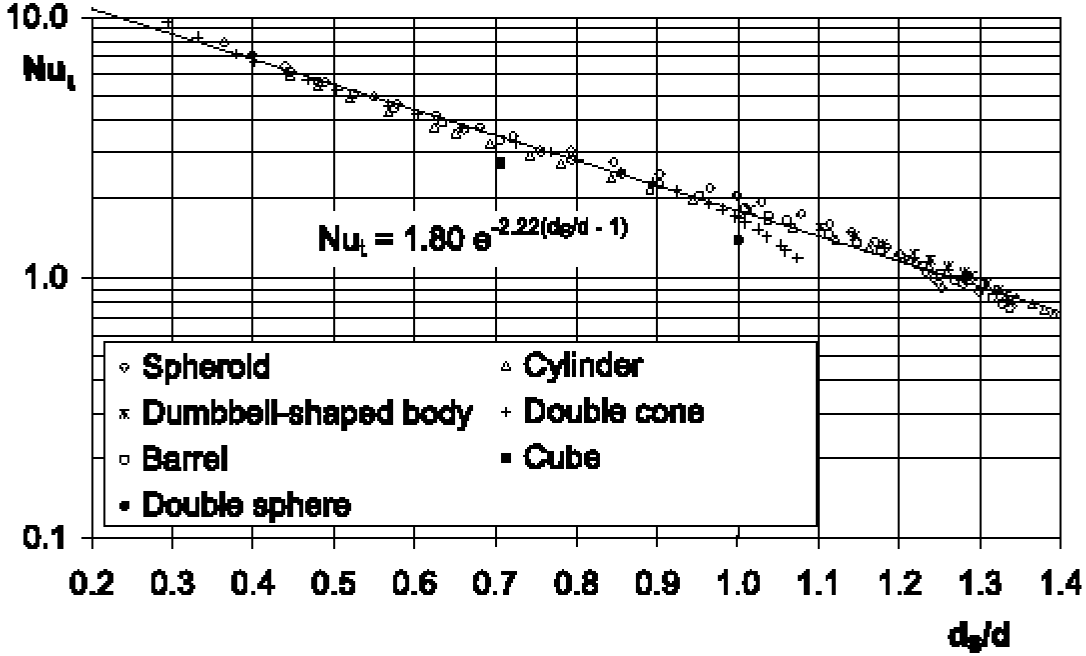
$$S_{de} = 2pb^2 + \frac{pa^2}{e}\ln\frac{1+e}{1-e}$$

$$S_{de} = 2pb^2 + \frac{2pab}{e}\arcsin(e)$$

$$j\left(\frac{a}{R}\right) = \frac{S_{de}}{S_{ds}}$$

$$\dot{Q} = j\left(\frac{a}{R}\right)S_{ds}q$$

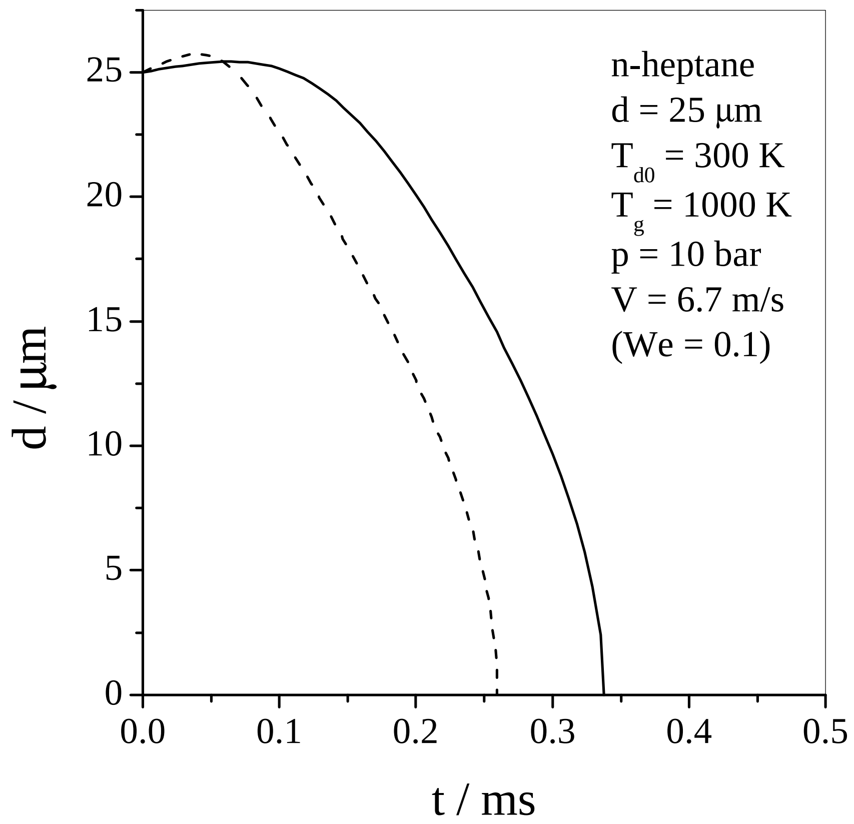
Variation of heat transfer coefficient

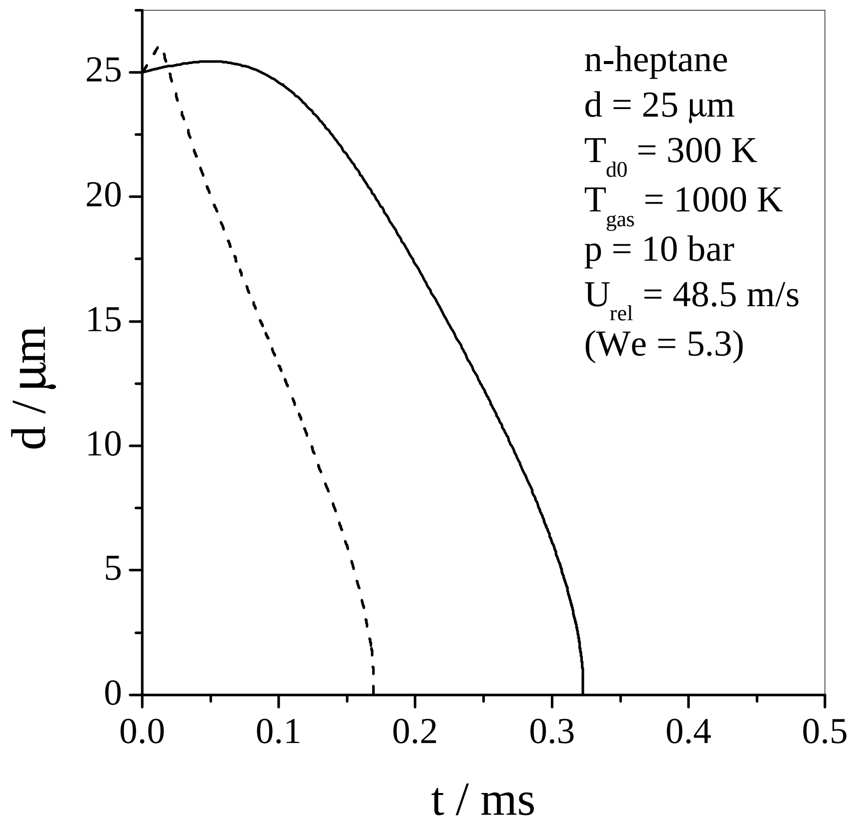


Wadewitz A., Specht E. (2001)

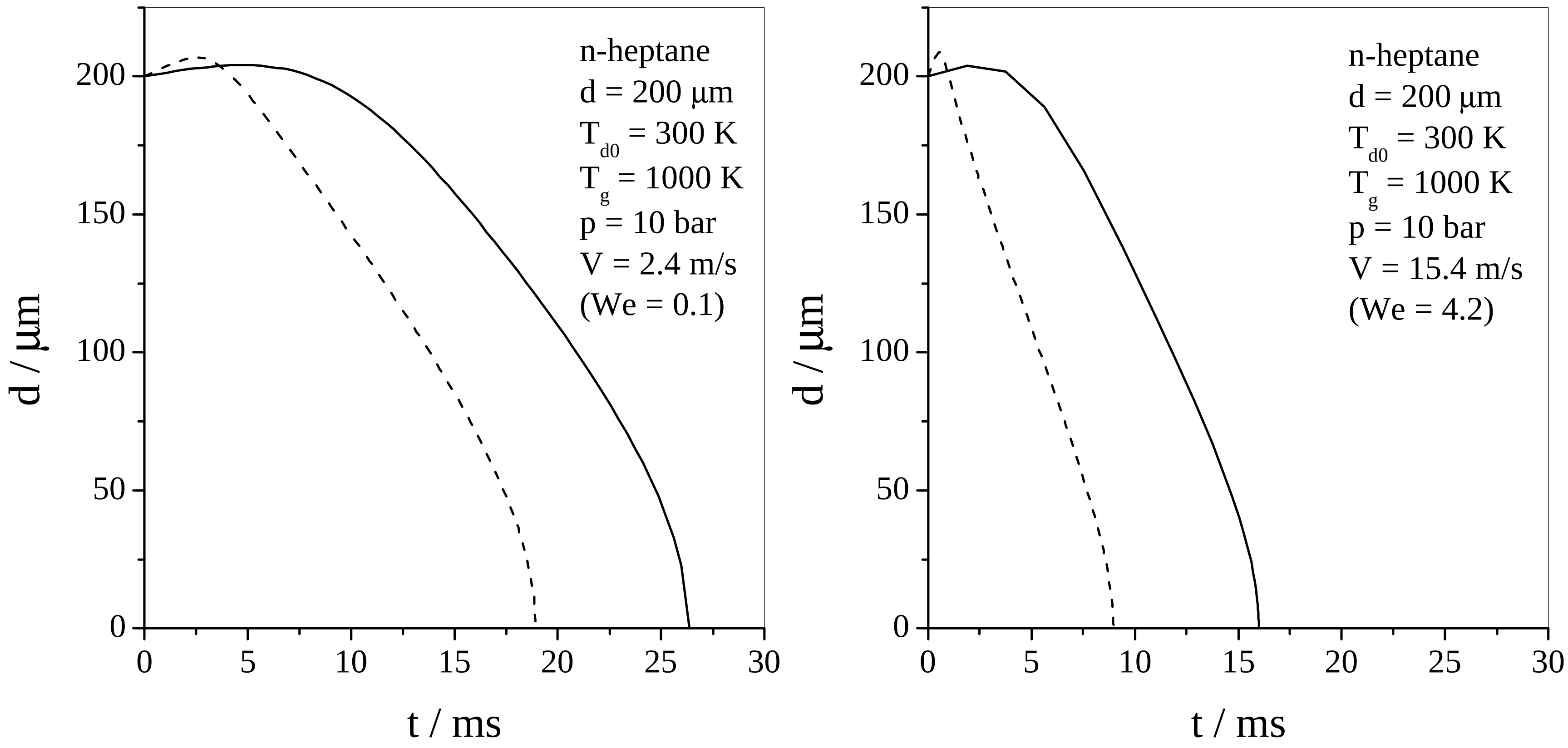
$$\frac{\mathrm{Nu}_q}{\mathrm{Nu}_{sq}} = \exp\left[-2.22\left(\frac{d_S}{d} - 1\right)\right]$$

Results of sample calculations I





Results of sample calculations II



Correction factors of the second group

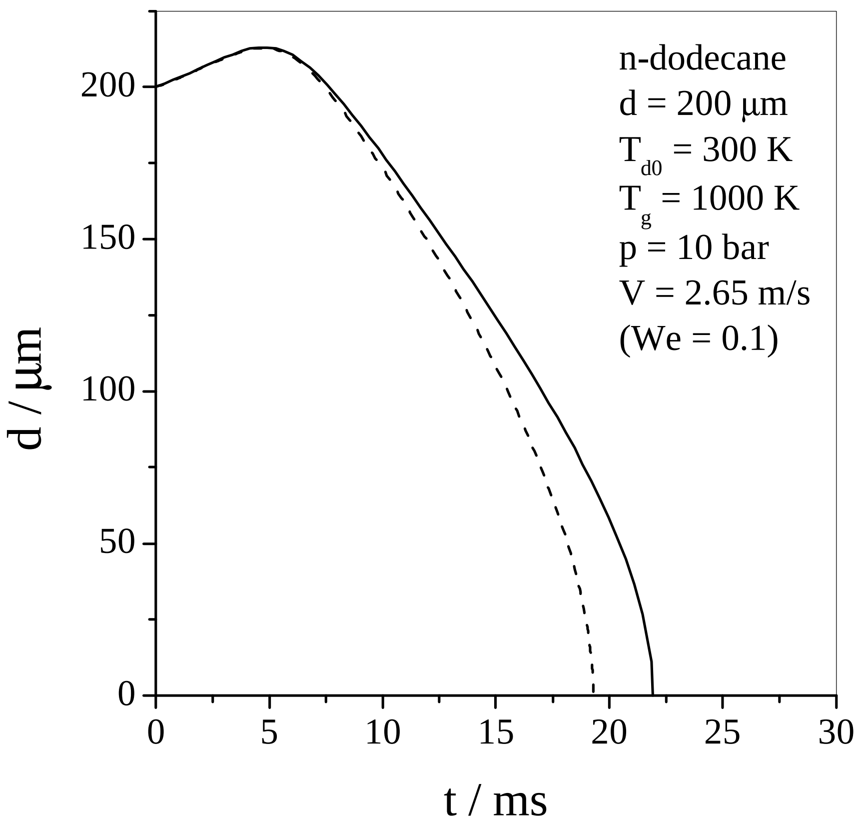
$$\frac{A}{A_s} = \frac{b^2}{R^2} = \left(1 + C_b y\right)^2$$

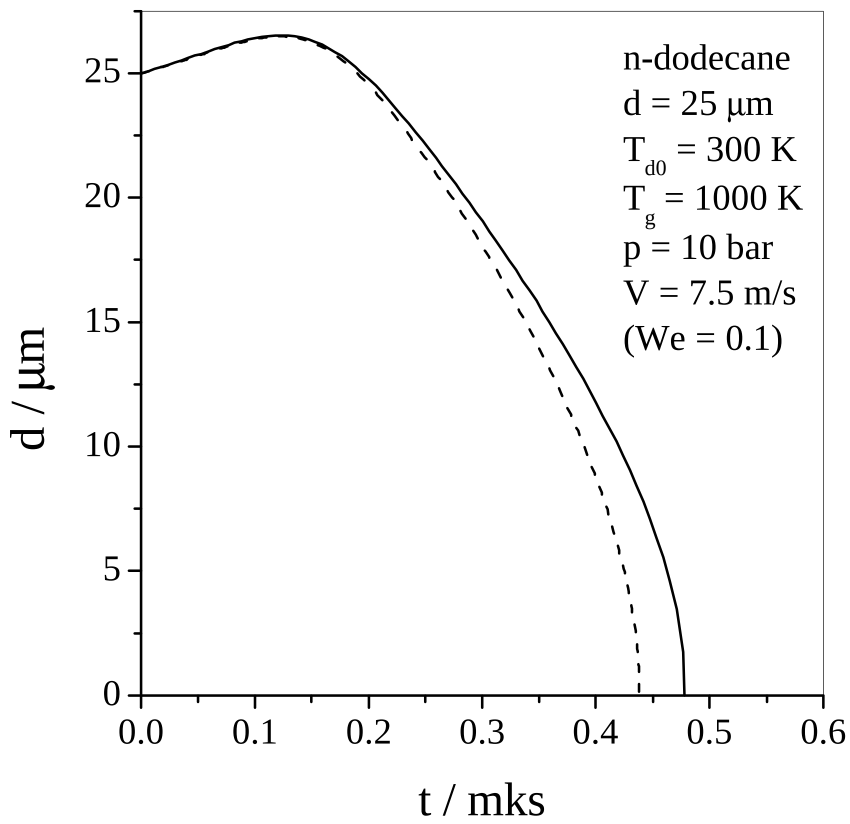
$$C_D = C_{Ds}(1 + 2.632y)$$

$$\frac{C_D}{C_{Ds}} = \left(\frac{2 + 3m_d / m_g}{3 + 3m_d / m_g}\right)\left(1 - 0.03\frac{m_g}{m_d}\mathrm{Re}_g^{0.65}\right)$$

$$C_D = \frac{C_{Ds}}{1 + B}$$

Results of sample calculations





Model II:
Transient heat and mass transfer

Energy balance equation for drop

?

$$c_l m_d \frac{dT_d}{dt} = \dot{Q}$$

$$\dot{Q} = A_d q = A_d a \left(T_g - T_d\right)$$

$$\frac{dT_d}{dt} - \frac{3}{2}\frac{Nu\, l_g}{r_l c_l r_d^2}\left(T_g - T_d\right) = 0$$

$$t = 0: \quad T_d = T_{d0}$$

Implications

(1) $q = a\left(T_g - T_d\right) \longrightarrow q = a\left(T_g - T_{ds}\right)$

(2) Steady state heat transfer $\longrightarrow$ Transient heat transfer

At Nu=2

$$T = T_g + \frac{r_d}{r}\left(T_{ds} - T_g\right)\left[1 - erf\left(\frac{r - r_d}{2\sqrt{\frac{l_g t}{r_g c_{pg}}}}\right)\right]$$

Sazhin (2001)

$$q = l_g \frac{\partial T}{\partial r} = l_g \frac{T_g - T_{ds}}{r_s}\left(1 + \frac{r_d}{\sqrt{\frac{p\, l_g t}{r_g c_{pg}}}}\right)$$

$$l_{\text{eff}} = l_g\left(1 + j\right)$$

$$j = r_d \sqrt{\frac{r_g c_{pg}}{p\, l_g t}}$$

Problem formulation

$$m_d c_l \frac{dT_d}{dt} = \dot{Q} + L \frac{dm_d}{dt}$$

$$\frac{dm_d}{dt} = -pd^2 j$$

$$\dot{Q} = pd^2 a \left(T_g - \underline{T_d}\right)$$

$$a = \frac{Nu}{d} \underline{l_{\mathrm{eff}}} \frac{\ln(1+B)}{B}$$

$$\underline{j = 2 \frac{r_g D}{d} \ln(1+B)}$$

(No “reference” temperature)

$$B = \frac{Y_{vs} - Y_{v\infty}}{1 - Y_{vs}}$$

$$\mathrm{Nu} = 2 + 0.6\,\mathrm{Re}^{1/2}\,\mathrm{Pr}^{1/3}$$

$$l_{\mathrm{eff}} = l_g (1 + j)$$

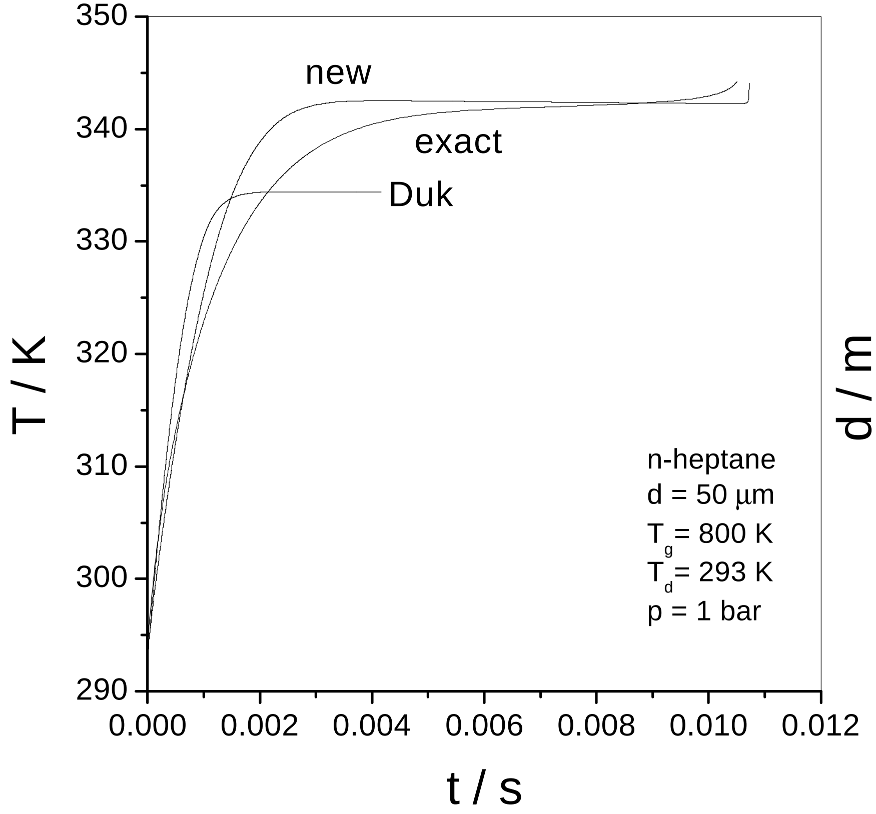
$$j = b r_d \sqrt{\frac{r_g c_{pg}}{p\, l_g t}}$$

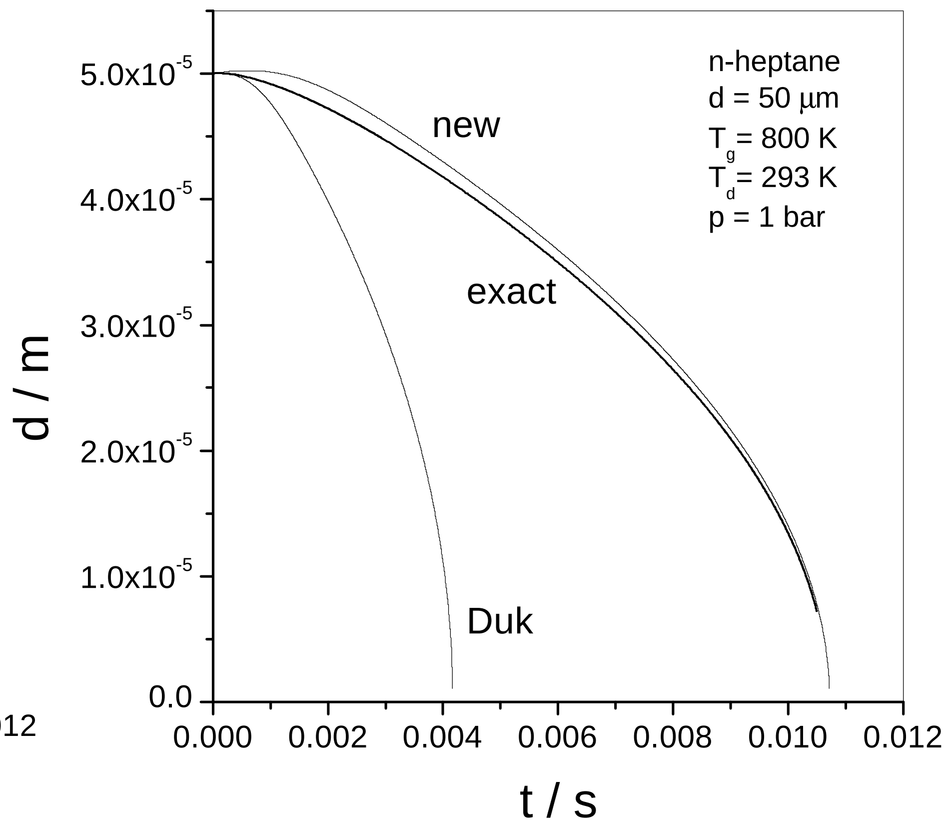
Initial conditions

$$T_d(0) = T_{d0} \qquad m_d(0) = m_{d0}$$

Model implementation

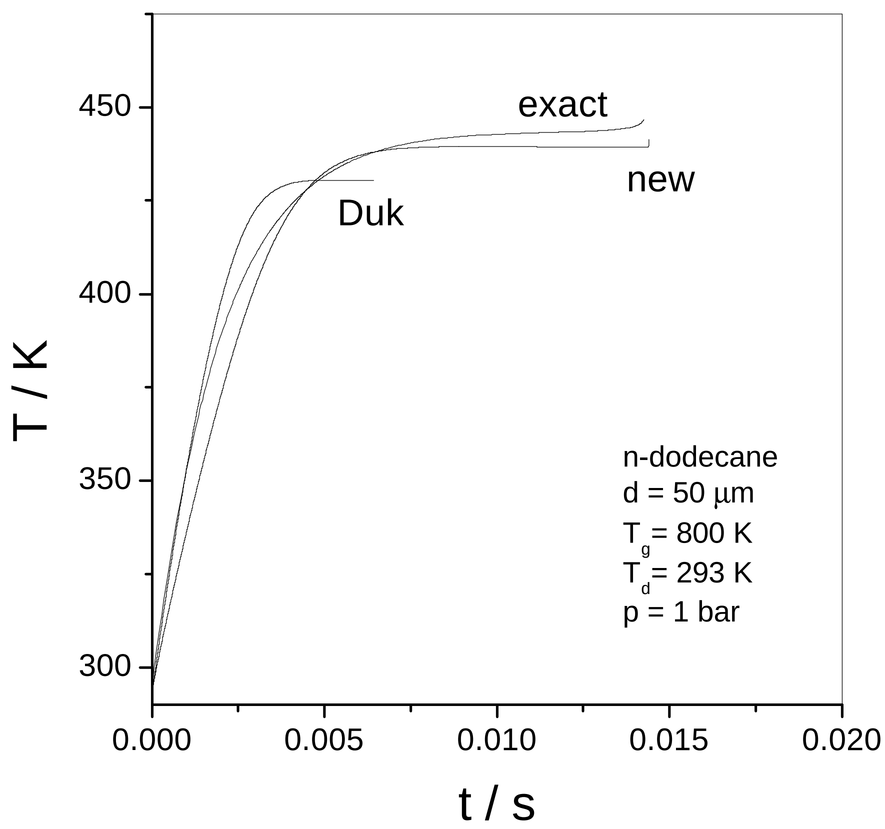
n-heptane, 1 bar

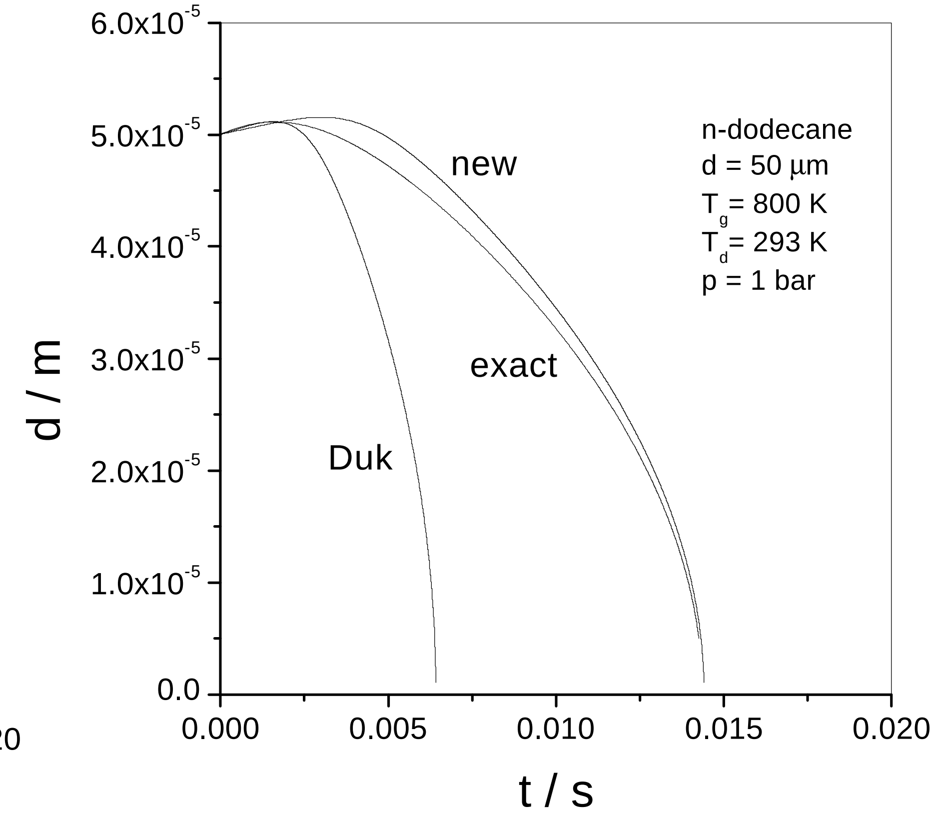




800 K

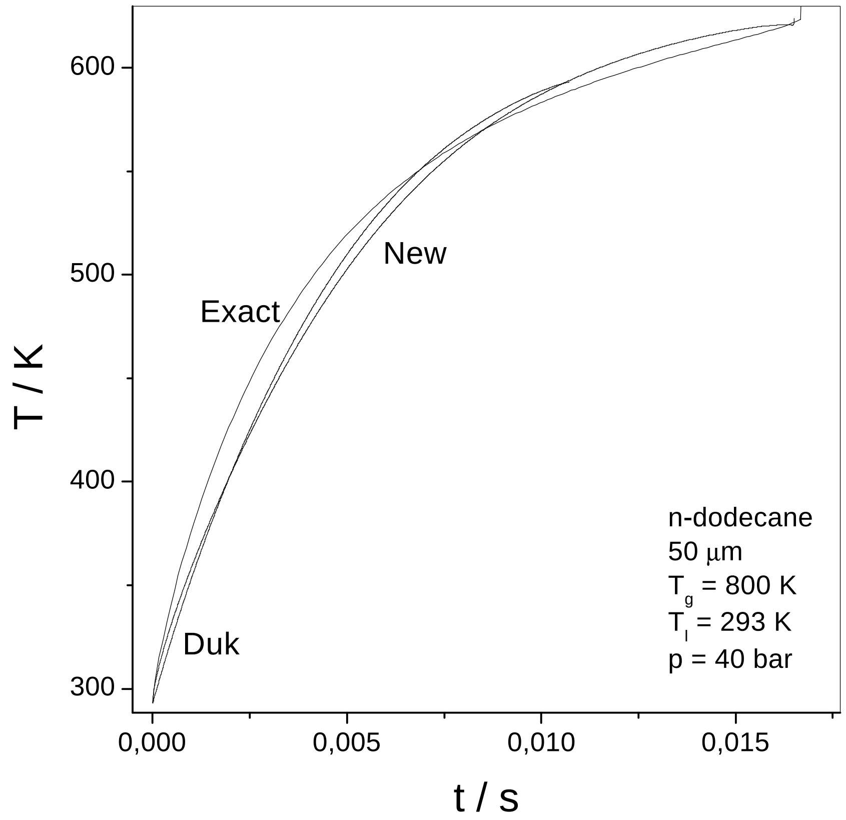
n-dodecane, 1 bar

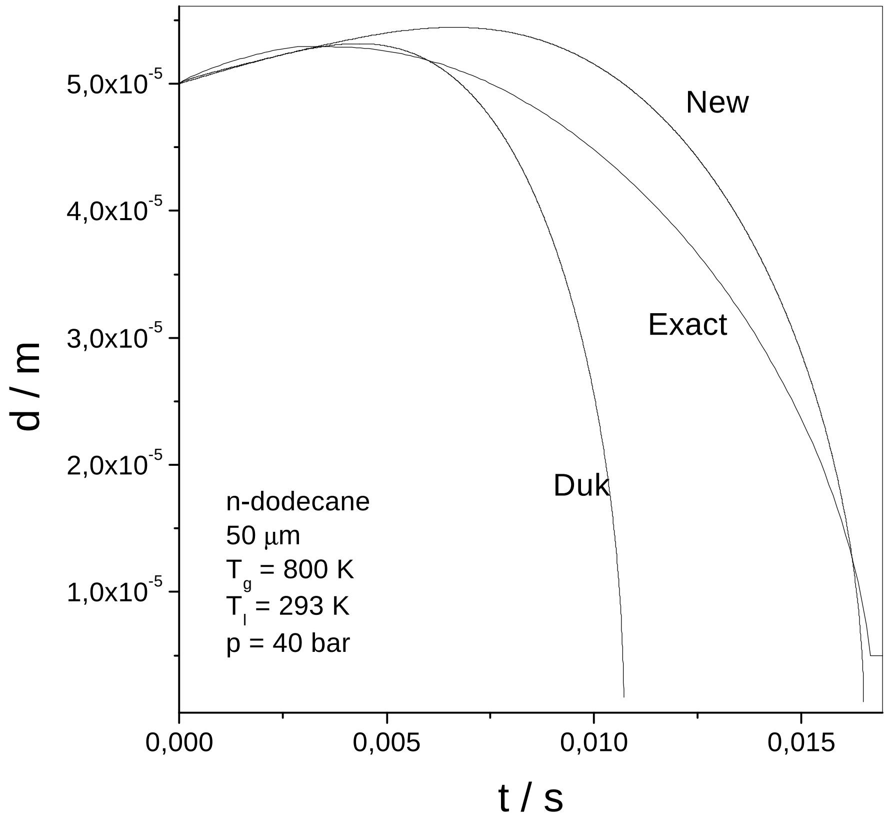




800 K

n-dodecane, 40 bar





800 K

Correction for nonuniform temperature distribution in the drop

Analytical solution for a spherical body of constant radius $r_d = const$

$$T_{dc} = T_{ds} + 2\left(T_{ds} - T_{d0}\right) \sum_{m=1}^{\infty} (-1)^m \exp\left(-pm \frac{at}{r_d^2} \right)$$

Analysis of numerical solution:

$$T_d \approx T_{dc} + \frac{3}{4}\left(T_{ds} - T_{dc}\right)$$

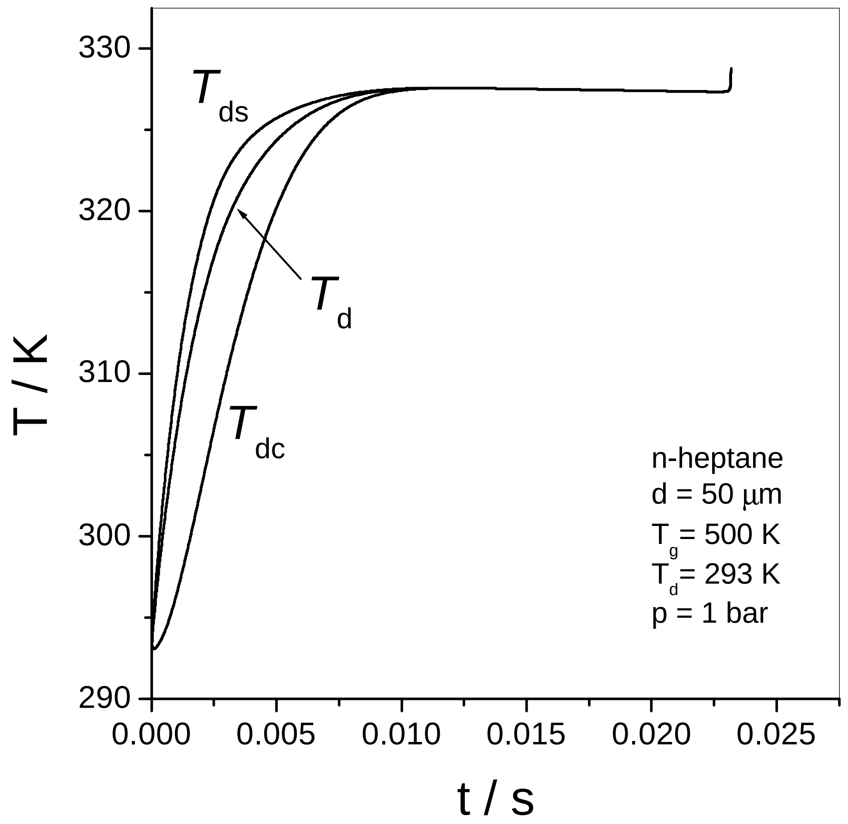
Drop surface temperature:

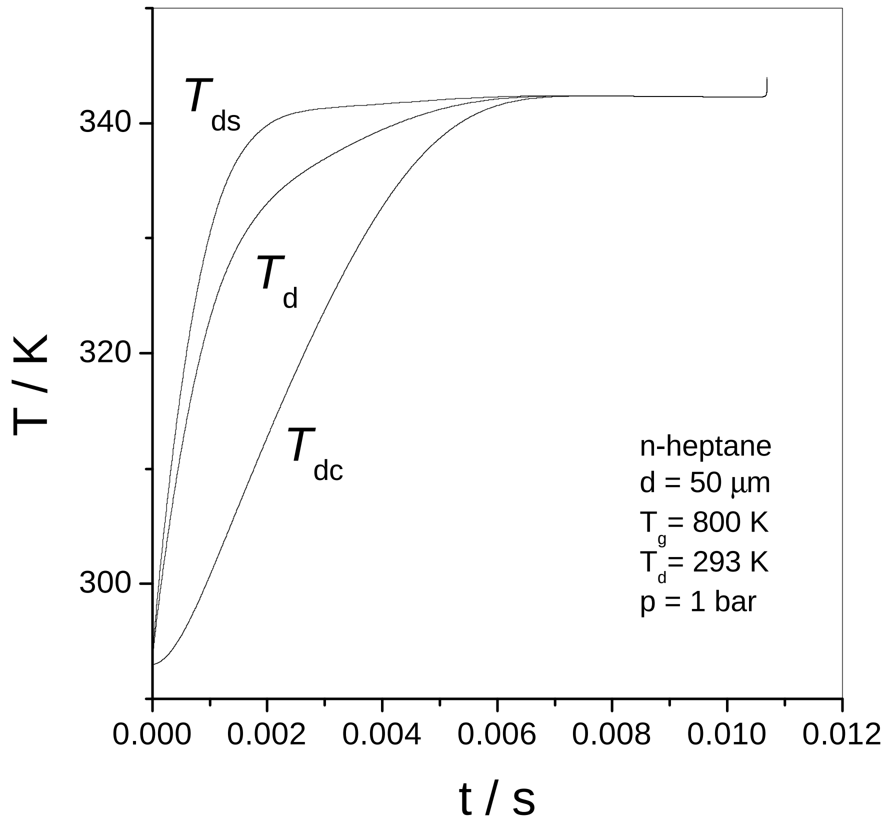
$$T_{ds} \approx \frac{4}{3} T_d - \frac{1}{3} T_{dc}$$

All physical properties are related to drop surface temperature !

Model II implementation

n-heptane, 1 bar

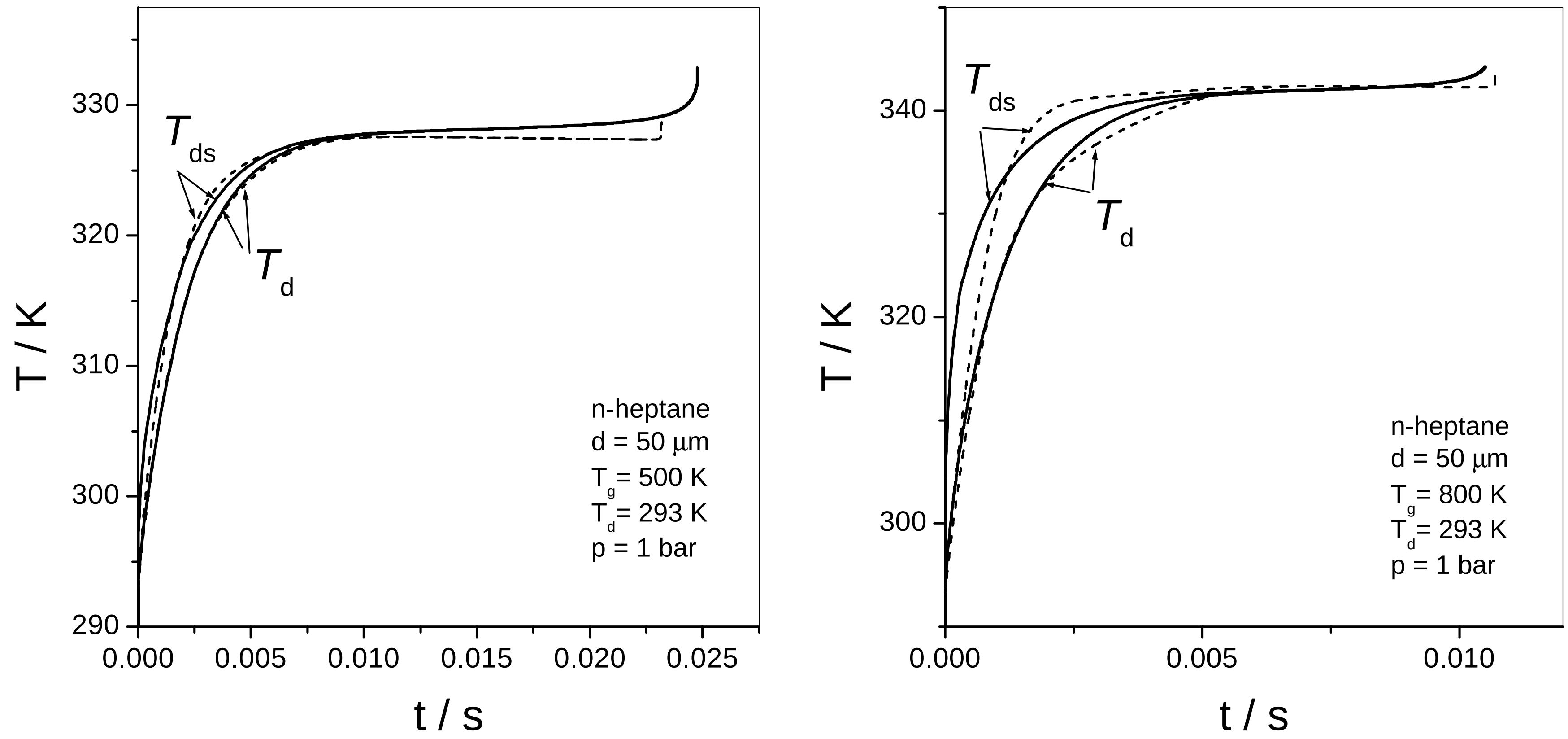




500 K **800 K**

Comparison with detailed model

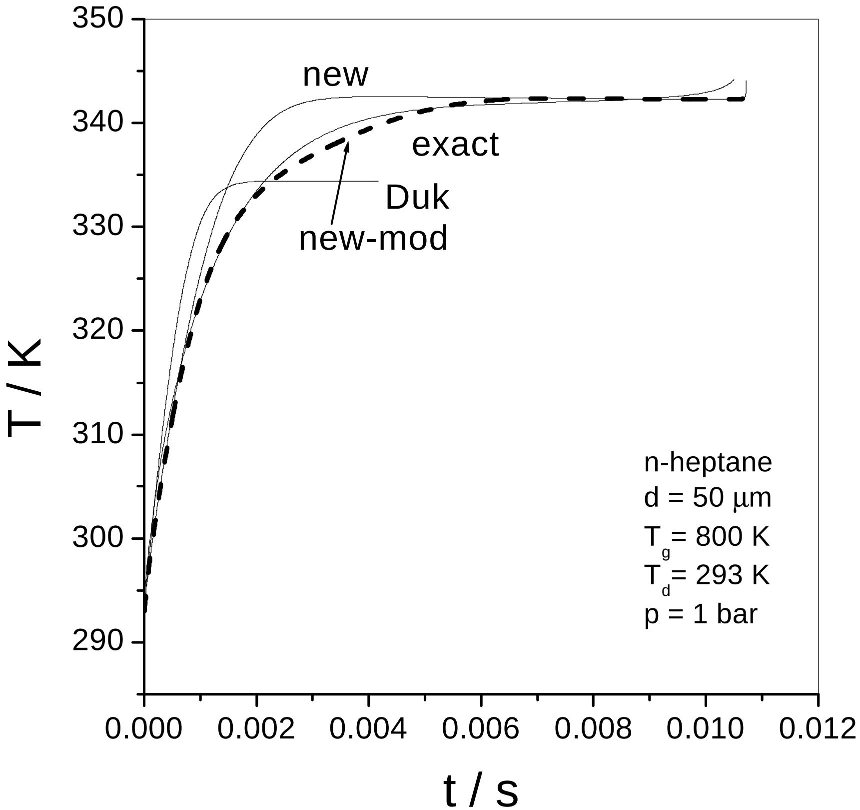
n-heptane, 1 bar

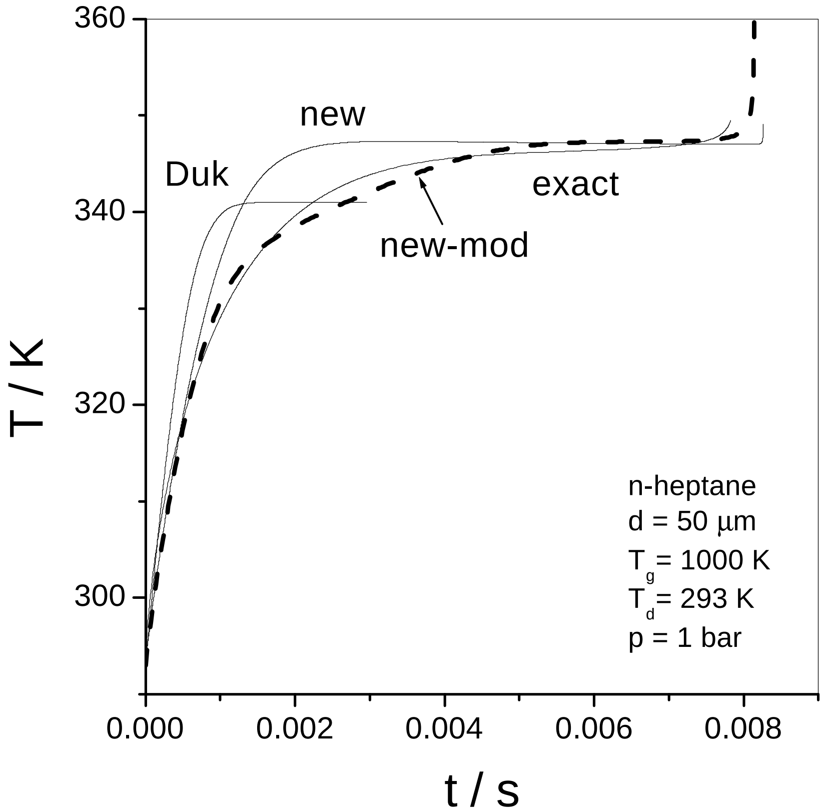


500 K **800 K**

Comparison between models

n-heptane, 1 bar





800 K **1000 K**

Conclusions

- Two new drop evaporation models
- Model I: correction factors taking into account internal liquid circulation and drop deformation
- Model II: Transient heat and mass transfer
- No Lewis number limitations
- Good prediction of ‘wet bulb’ temperature
- Good prediction of drop lifetime
- Possibility of user interference
- No increase in the CPU time