

# The Sir Harry Ricardo Laboratories

## Modelling Of Spray and Film Drying: Preliminary Results

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# Plan

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- Basic equations (film)
- Preliminary results

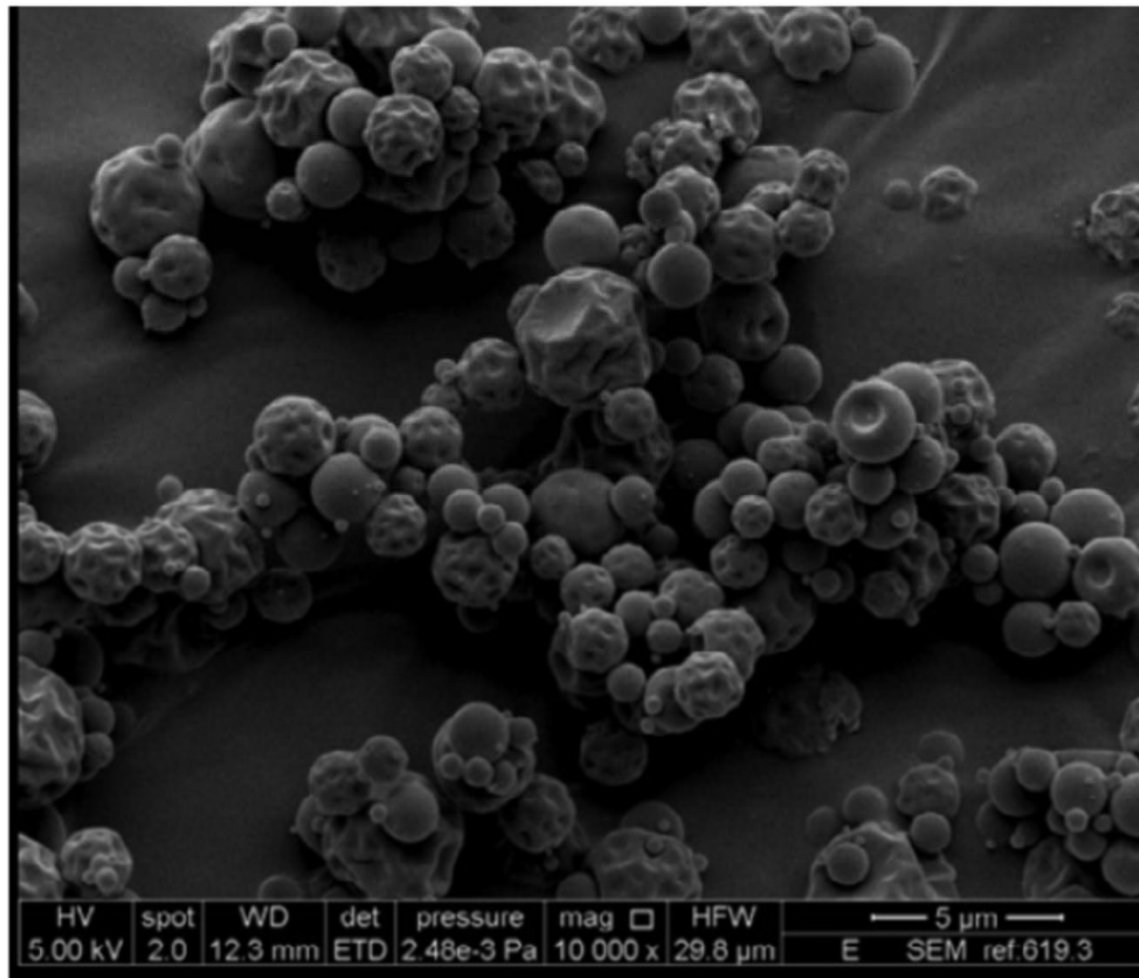
# Background

## Background

Chitosan (polymer) was weighed on a high accuracy analytical balance and dissolved in de-ionized water. The solution was spray-dried using a lab-scale nanospray dryer equipped with a piezoelectrically driven droplet atomizing technology. The inlet temperature was 120 C, pump flow rate 20 mL/h, gas flow rate 133 L/min, 5.5  $\mu\text{m}$  mesh nozzle and instrument pressure 47 mbar. Spray-dried powders were immediately transferred to a glass vial and kept in a desiccator to prevent crystallization.

The shape and surface morphology of the spray-dried chitosan powder was examined using scanning electron microscopy (SEM) (FEI Quanta 200F SEM; Eindhoven, Netherlands). Samples were prepared by placing a small amount of freshly spray-dried powder on an aluminium specimen pin covered with double-sided adhesive carbon tabs (Agor Scientific, UK) followed by sputter coating with gold (Quorum Q150R; Quorum Technologies Ltd., UK) prior to observation under SEM. A typical SEM micrograph for spray-dried chitosan particles is shown in Fig. 1

## Background



## Basic equations (droplet)

### Conduction limit. Effective conductivity

$$c_1 \rho_1 \frac{\partial T}{\partial t} = k_1 \left( \frac{\partial^2 T}{\partial R^2} + \frac{2}{R} \frac{\partial T}{\partial R} \right) + P(R)$$

$$h(T_g - T_s) = -\rho_1 L \dot{R}_d + k_1 \frac{\partial T}{\partial R} \Big|_{R=R_d}$$

$$k_{\text{eff}} = \chi_T k_l, \quad T_{\text{eff}} = T_g + \frac{\rho_1 L \dot{R}_d}{h}$$

where the coefficient  $\chi_T$  varies from about 1 (at droplet Peclet number  $\text{Pe}_{d(l)} = \text{Re}_{d(l)} \text{Pr}_l < 10$ ) to 2.72 (at  $\text{Pe}_{d(l)} > 500$ ) and can be approximated as

$$\chi_T = 1.86 + 0.86 \tanh [2.225 \log_{10} (\text{Pe}_{d(l)} / 30)].$$

## Analytical solution for $h=\text{const}$

$$T(R,t) = \frac{R_d}{R} \sum_{n=1}^{\infty} \left[ q_n \exp[-\kappa_R \lambda_n^2 t] - \frac{\sin \lambda_n}{||v_n||^2 \lambda_n^2} \mu_0(0) \exp[-\kappa_R \lambda_n^2 t] \right. \\ \left. - \frac{\sin \lambda_n}{||v_n||^2 \lambda_n^2} \int_0^t \frac{d\mu_0}{d\tau} \exp[-\kappa_R \lambda_n^2 (t - \tau)] d\tau \right] \sin \left[ \lambda_n \left( \frac{R}{R_d} \right) \right] + T_g(t)$$

where  $\lambda_n$  are solutions to the equation:  $\lambda \cos \lambda + h_0 \sin \lambda = 0$ ,

$$||v_n||^2 = \frac{1}{2} \left( 1 - \frac{\sin 2\lambda_n}{2\lambda_n} \right) = \frac{1}{2} \left( 1 + \frac{h_0}{h_0^2 + \lambda_n^2} \right), \quad \kappa_R = \frac{k_l}{c_l \rho_l R_d^2}$$

$$q_n = \frac{1}{R_d ||v_n||^2} \int_0^{R_d} \hat{T}_0(R) \sin \left[ \lambda_n \left( \frac{R}{R_d} \right) \right] dR,$$

$$h_0 = \frac{h R_d}{k_l} - 1 \quad \hat{T}_0(R) = \frac{RT_{d0}(R)}{R_d} \quad \mu_0(t) = \frac{h T_g(t) R_d}{k_l}$$

The effect of thermal radiation is not taken into account in this solution.



## Discrete components model

$$\frac{\partial Y_{li}}{\partial t} = D_{\text{eff}} \left( \frac{\partial^2 Y_{li}}{\partial R^2} + \frac{2}{R} \frac{\partial Y_{li}}{\partial R} \right)$$

Boundary and initial conditions:

$$\alpha(\epsilon_i - Y_{lis}) = D_{\text{eff}} \frac{\partial Y_{li}}{\partial R} \Big|_{R=R_R-0}$$

$$\frac{\partial Y_{li}}{\partial R} \Big|_{R=0} = 0; \quad Y_{li}(t=0) = Y_{li0}(R); \quad R \leq R_d$$

Effective diffusivity  $D_{\text{eff}} = \chi_Y D_l$  where  $\chi_Y = 1.86 + 0.86 \tanh [2.225 \log_{10}(\text{Pe}_{dY}/30)]$

$\chi_Y$  increases from 1 to 2.72 when  $\text{Pe}_{dY} = \text{Re}_d \text{Sc}$  increases from  $<10$  to  $> 500$

$\text{Sc} = \nu_l / D_l$  is the liquid Schmidt number;  $\epsilon_i = \frac{Y_{vis}}{\sum_i Y_{vis}}$   $\alpha = \frac{|\dot{m}_d|}{4\pi\rho_l R_d^2}$

### Discrete components model

*Equation for the partial fuel vapour pressures at the surface of the droplet*

$$p_{vis} = \gamma_i X_{lis} p_{vis}^*$$

where  $X_{lis}$  is the molar fraction of the  $i$ th species in the liquid near the droplet surface,  $p_{vis}^*$  is the partial vapour pressure of the  $i$ th species in the case  $X_{lis} = 1$ ,  $\gamma_i$  is the activity coefficient. In some applications, the latter coefficient can be assumed equal to 1. In this case, this equation leads to the Raoult law

## Analytical solution to the species diffusion equation

$$Y_{li}(R,t) = \epsilon_i + \frac{1}{R} \left\{ \exp \left[ -D_{\text{eff}} \left( \frac{\lambda_0^2}{R_d^2} \right) t \right] [q_{Yi0} - \epsilon_i(0) Q_{Y0}] \sinh \left[ \lambda_0 \left( \frac{R}{R_d} \right) \right] \right. \\ \left. + \sum_{n=1}^{\infty} \left\{ \exp \left[ -D_{\text{eff}} \left( \frac{\lambda_n^2}{R_d^2} \right) t \right] [q_{Yin} - \epsilon_i(0) Q_{Yn}] \sin \left[ \lambda_n \left( \frac{R}{R_d} \right) \right] \right\} \right\}$$

where  $\lambda_n$  are solutions to the equations:  $\lambda \cosh \lambda + h_{Y0} \sinh \lambda = 0$  ( $n = 0$ ),  $\lambda \cos \lambda + h_{Y0} \sin \lambda = 0$  ( $n \geq 1$ ),

$$\|v_{Yn}\|^2 = -\frac{R_d}{2} \left( 1 + \frac{h_{Y0}}{h_{Y0}^2 - \lambda_0^2} \right), \quad \|v_{Yn}\|^2 = \frac{R_d}{2} \left( 1 + \frac{h_0}{h_0^2 + \lambda_n^2} \right) \quad (n \geq 1),$$

$$q_{Yn} = \frac{1}{\|v_{Yn}\|^2} \int_0^{R_d} v_{Yn}^2(R) dR,$$

$$h_{Y0} = - \left( 1 + \frac{\alpha R_d}{D_{\text{eff}}} \right)$$

$$\alpha = \frac{|\dot{m}_d|}{4\pi \rho_l R_d^2}$$

$$Q_{Yn} = \begin{cases} -\frac{1}{\|v_{Y0}\|^2} \left( \frac{R_d}{\lambda_0} \right)^2 (1 + h_{Y0}) \sinh \lambda_0 & \text{when } n = 0 \\ \frac{1}{\|v_{Yn}\|^2} \left( \frac{R_d}{\lambda_n} \right)^2 (1 + h_{Y0}) \sin \lambda_n & \text{when } n \geq 1 \end{cases}$$

## Basic equations (film)

## Basic equations (temperature)

$$\frac{\partial T}{\partial t} = \kappa_l \frac{\partial^2 T}{\partial x^2}$$

$$h(T_{\text{eff}} - T_s) = k_l \left. \frac{\partial T}{\partial x} \right|_{x=\delta_0-0}$$

$$T_{\text{eff}} = T_g + \frac{\rho_l L \dot{\delta}_{0e}}{h},$$

## Basic equations (temperature)

$$T(X, t) = T_w + \frac{X h_0}{1 + h_0} (T_{\text{eff}} - T_w) + \sum_{n=1}^{\infty} \exp [-\kappa_{\delta 0} \lambda_n^2 t] [q_n + f_n h_0 (T_{\text{eff}} - T_w)] \sin(\lambda_n X), \quad (4)$$

where  $X = x/\delta_0$ ,  $h_0 = h\delta_0/k_l$ ,  $\kappa_{\delta 0} = k_l/(c_l \rho_l \delta_0^2)$ ,

$$q_n = \frac{1}{\|v_n\|^2} \int_0^1 (T_0(X) - T_w) \sin(\lambda_n X) dX, \quad f_n = \frac{1}{\|v_n\|^2} \int_0^1 f(X) \sin(\lambda_n X) dX = -\frac{\sin \lambda_n}{\|v_n\|^2 \lambda_n^2},$$

$f(X) = -X/(1+h_0)$ ,  $\|v_n\|^2 = \frac{1}{2} \left(1 - \frac{\sin 2\lambda_n}{2\lambda_n}\right) = \frac{1}{2} \left(1 + \frac{h_0}{h_0^2 + \lambda_n^2}\right)$ ,  $\lambda_n$  are non-trivial solutions to the equation

$$\lambda \cos \lambda + h_0 \sin \lambda = 0. \quad (5)$$

## Basic equations (species mass fractions)

$$\frac{\partial Y_{l,i}}{\partial t} = D_l \frac{\partial^2 Y_{l,i}}{\partial x^2}$$

$$D_l \frac{\partial Y_{l,i}}{\partial x} \Big|_{x=\delta_0-0} = |\dot{\delta}_{0e}| (Y_{l,i}|_{x=\delta_0} - \epsilon_i),$$

$$\frac{\partial Y_{l,i}}{\partial x} \Big|_{x=0} = 0,$$

## Basic equations (species mass fractions)

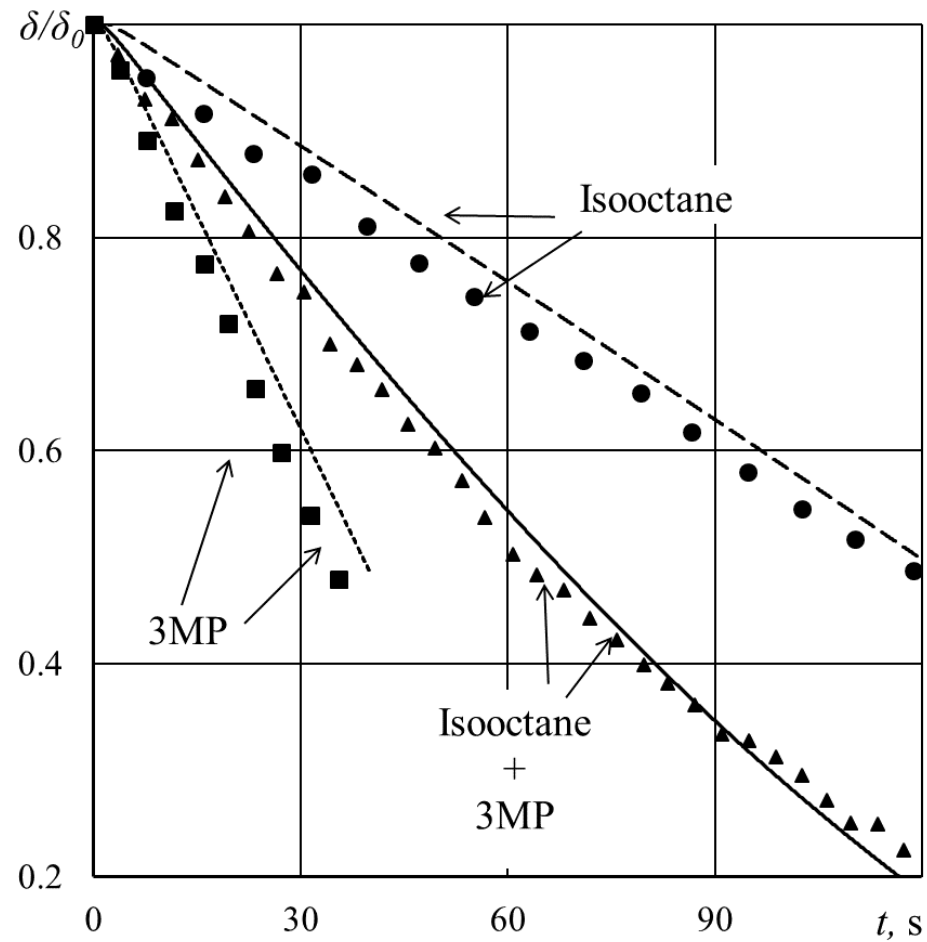
$$Y_{vs,i}(t, x) = q_0 \exp \left[ D_l \left( \frac{\lambda_0}{\delta_0} \right)^2 t \right] \cosh \left( \lambda_0 \frac{x}{\delta_0} \right) + \sum_{n=1}^{\infty} q_n \exp \left[ -D_l \left( \frac{\lambda_n}{\delta_0} \right)^2 t \right] \cos \left( \lambda_n \frac{x}{\delta_0} \right) + \epsilon_i$$

Raoult law

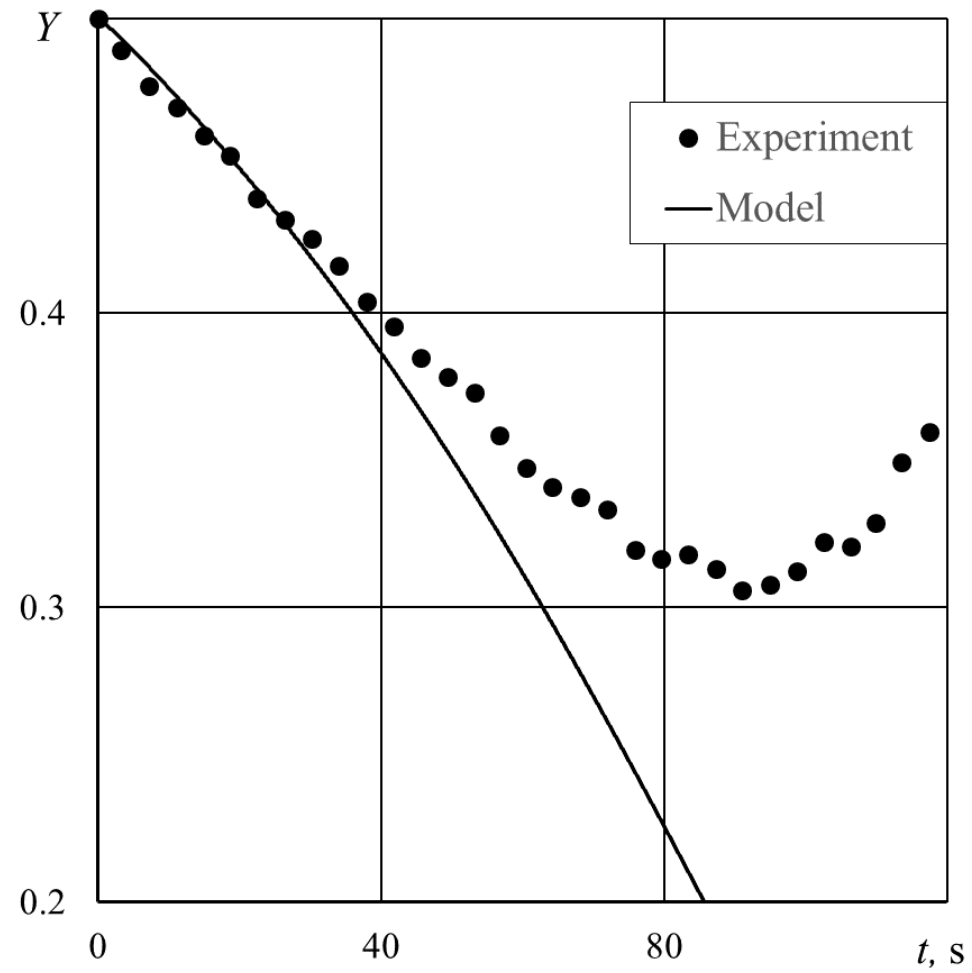
$$p_{vs,i} = X_{ls,i} p_{v,i}^*$$



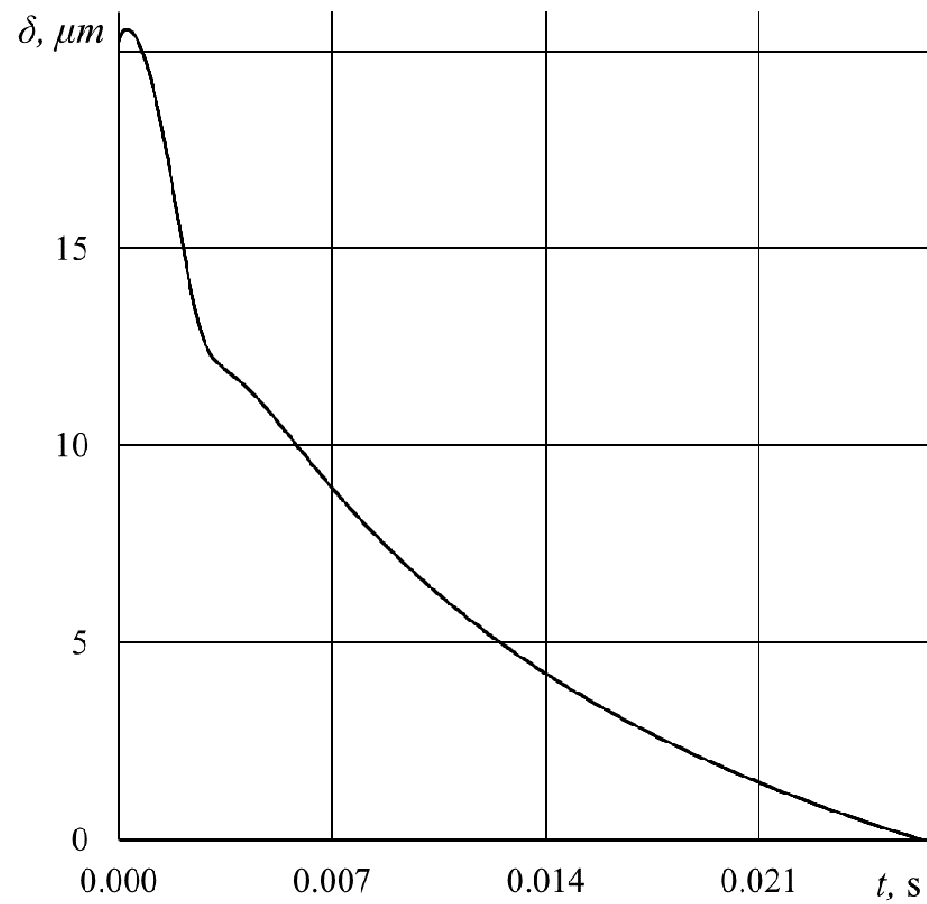
## Preliminary results (film)



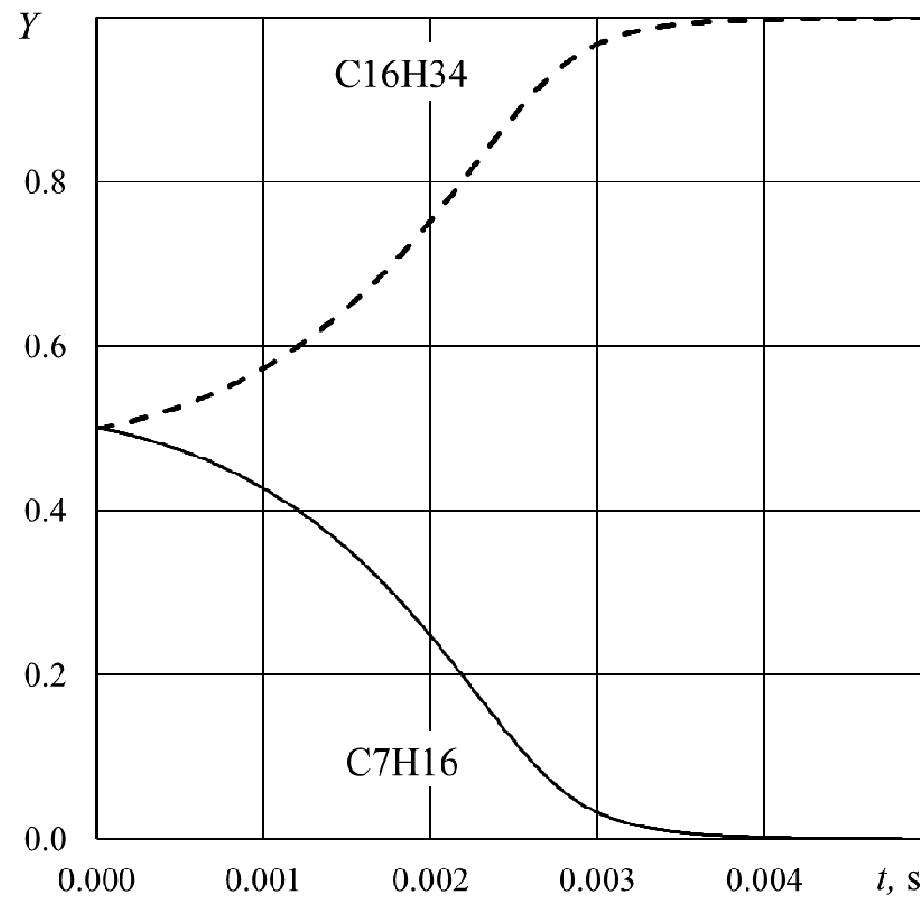
## Preliminary results (film)



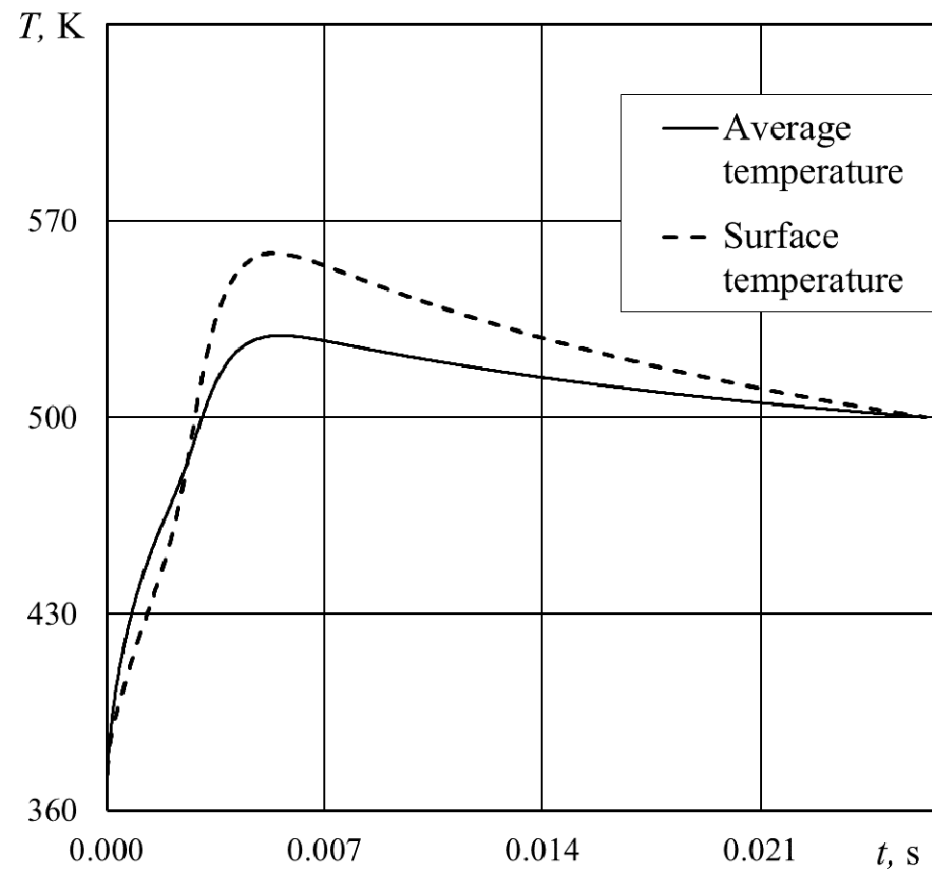
## Preliminary results (film)



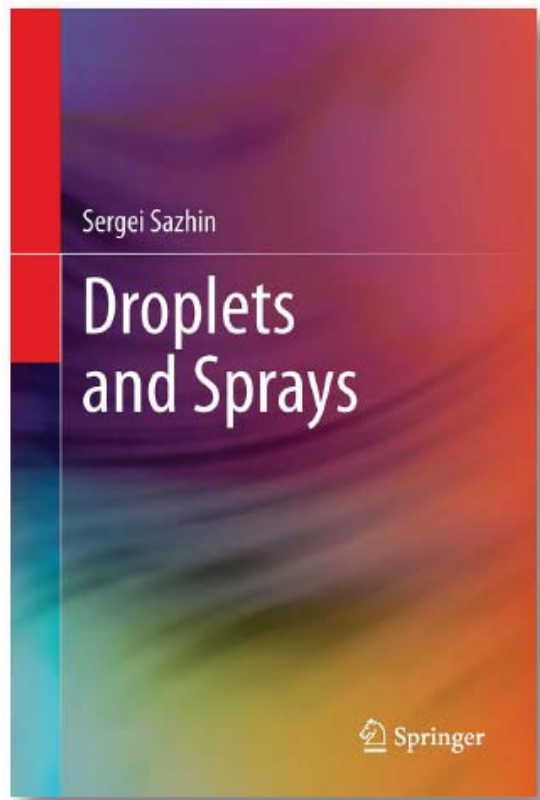
## Preliminary results (film)



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# Challenges referring to spray modelling




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Review article

Modelling of fuel droplet heating and evaporation: Recent results and unsolved problems

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**Thank you for your attention**



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