Imperial College
London

Modelling of intensified transfer processes in thin liquid films

Omar K. Matar & Chris Lawrence
Department of Chemical Engineering

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outline

- background
- simple scaling
- hydrodynamics
    - integral method
    - travelling waves and full transient solutions
- diffusion (mass transfer)
    - 2D solutions
    - integral method
    - asymptotic method
- summary

background

- IMI project
- experiments

background – IMI project

- Innovative Manufacturing Initiative (EPSRC)
  - spinning disk reactor for desktop drug manufacture
- Newcastle University
  - experiments & equipment design
- Imperial
  - modelling and simulation
- industrial partners
  - Glaxo Wellcome (now GSK), Astra Zeneca
  - Hickson Welch (now C6 solutions), Thomas Swann, Robinson Brothers, AH Marks
  - Alfa Laval (replaced by Mettler Toledo), Rosand Engineering (now Triton)
  - Protensive Ltd

collaborators

- Omar Matar Chris Lawrence
  - Department of Chemical Engineering, Imperial College London
- Grigori Sisoev
  - Faculty of Mechanics and Mathematics Moscow M. V. Lomonosov State University

- John Burns, Colin Ramshaw, Roshan Jachuck
  - Protensive Ltd

spinning disc reactor

- replace large stirred tanks
  - batch process $\rightarrow$ continuous process
- bench-scale equipment
  - factory scale throughput
- close control over material history
  - thermal, chemical, mechanical
- high speed
  - low residence time, low inventory
- SDR generates a thin film
  - good heat transfer, mass transfer

flow visualisation

- 100 rpm

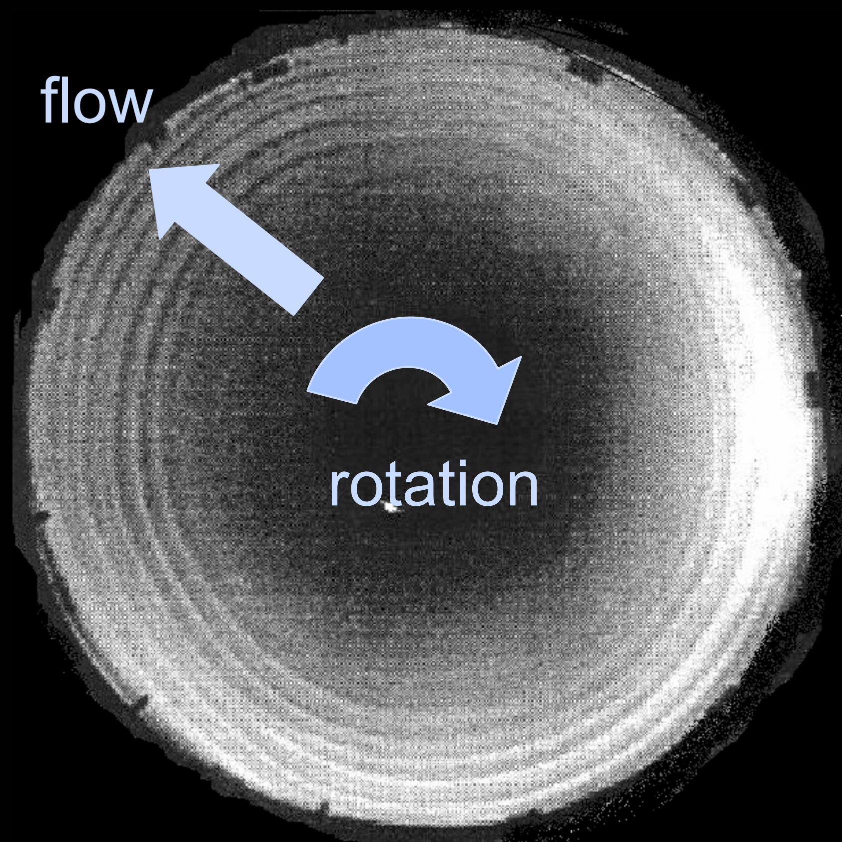


Figure 5.1(c): Variation of wavefronts across the disc,
$Q = 7$ cc/s, $\Omega = 100$ rpm.

flow visualisation

- 200 rpm

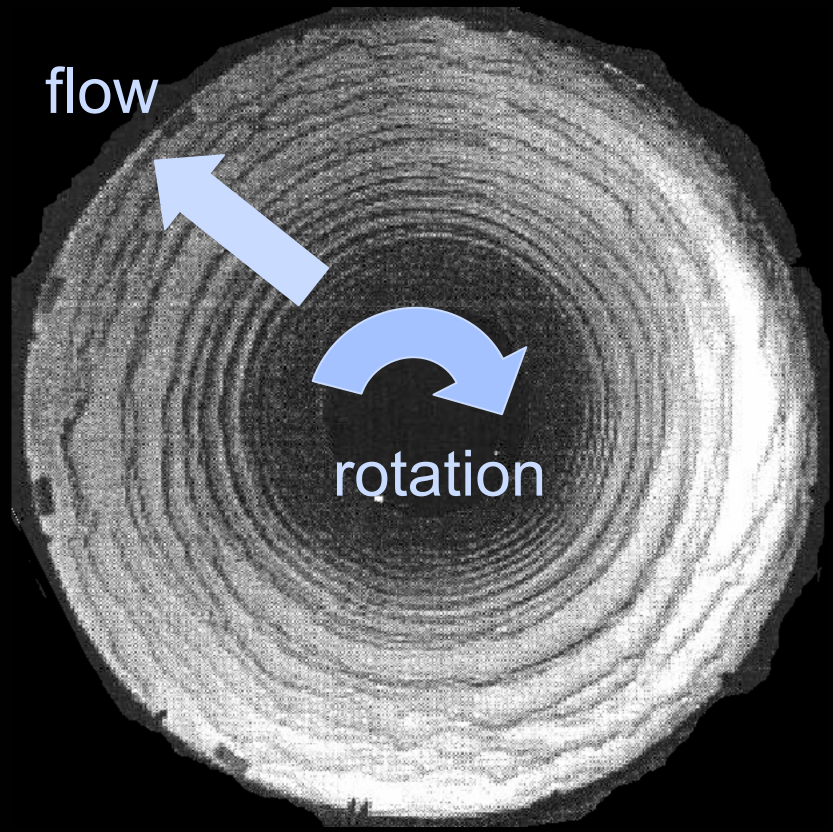
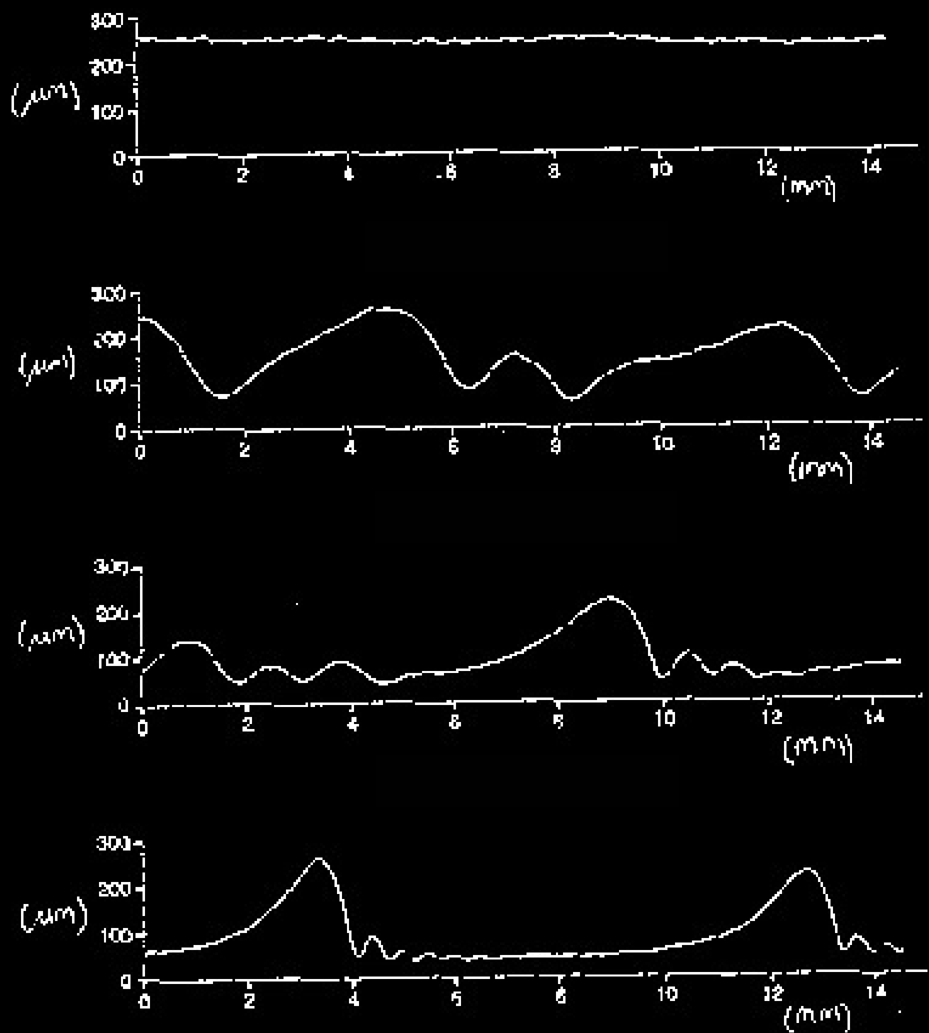


Figure 5.2(c): Variation of wavefronts across the disc,
$Q = 7$ cc/s, $\Omega = 200$ rpm.

wave profiles

flow



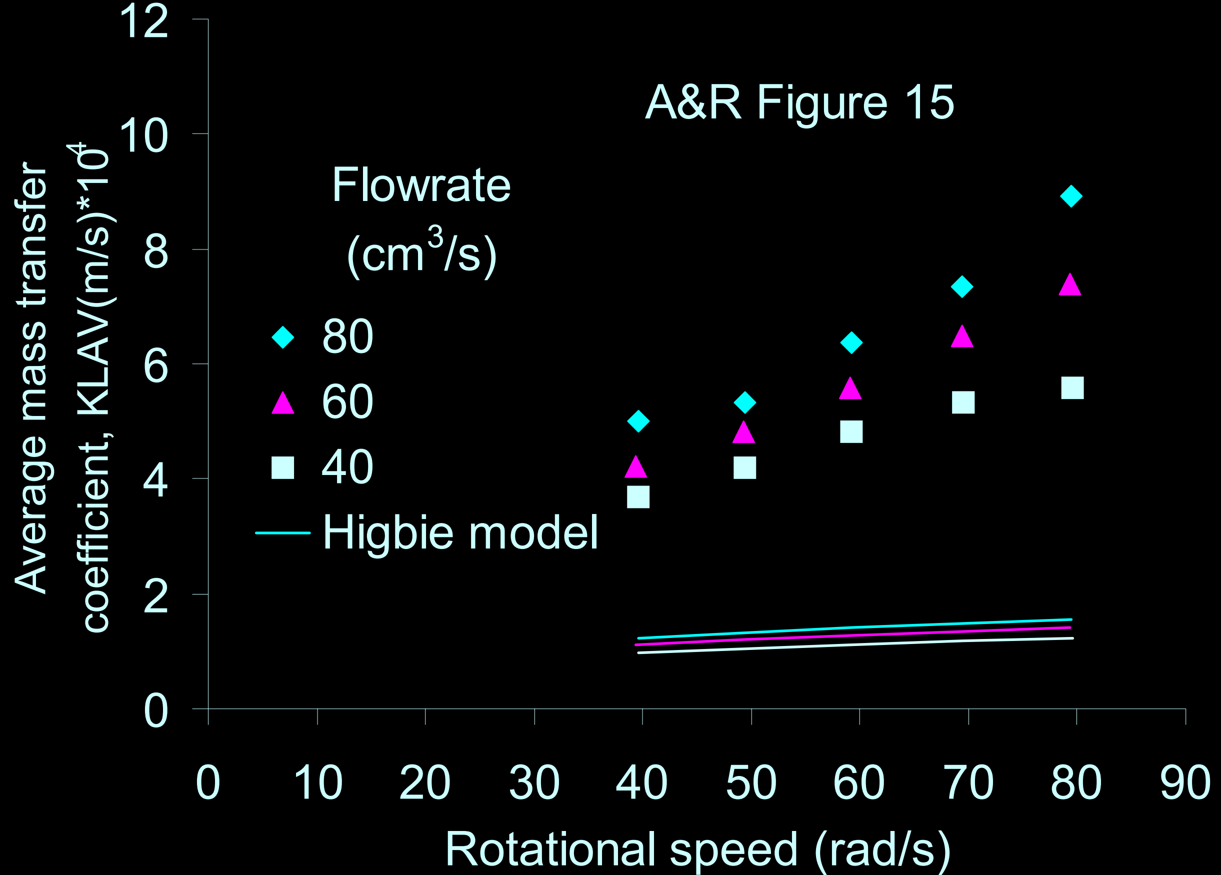
100 rpm

200 rpm

300 rpm

400 rpm

mass transfer enhancement



model approaches

- basic model
  - Nusselt (flow) + Higbie (mass transfer)
  - gives baseline
  - fails to capture enhancement
- scaling model
  - captures enhancement
  - does not explain
- detailed model
  - provides explanation and understanding

simple scaling

- operating parameters
  - Ω disc rotation speed (100 – 1000 rpm)
  - Q_C volume flow rate (10 – 100 cm^3/s)
  - R_{disk} disk radius (5 – 25 cm)
- fluid properties
  - ν kinematic viscosity (10^{-6} m^2/s)
  - ρ density (10^3 kg/m^3)
  - σ surface tension (0.07 N/m)
  - D solute diffusion coefficient (10^{-9} m^2/s)

scaling

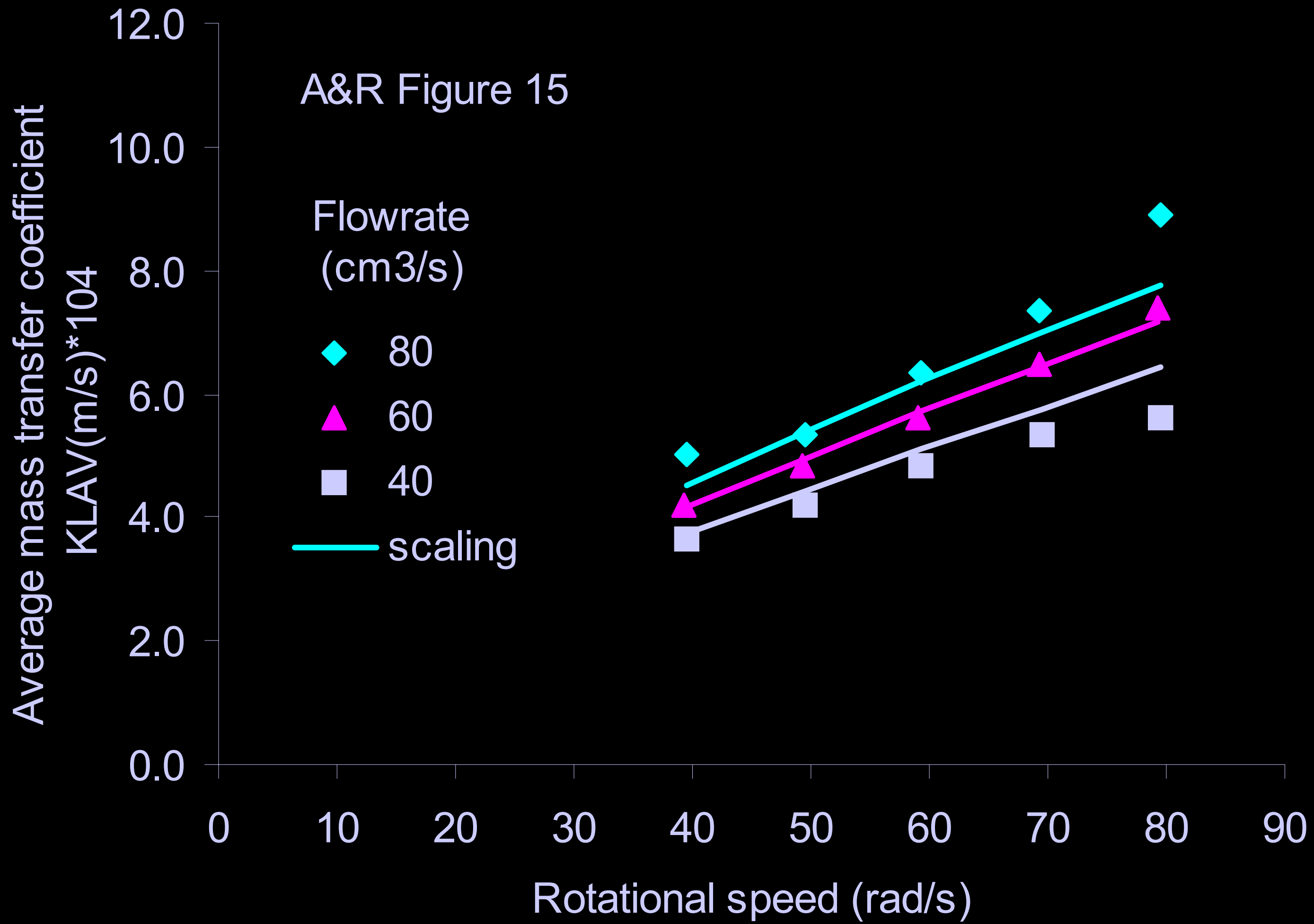
Nusselt scale $$H_C = \left(\frac{Q_C \nu}{2\pi \Omega^2 R_C^2} \right)^{1/3}$$

Peclet number $$Pe = \frac{\Omega^2 H_C^4}{\nu D}$$

wave parameter $$\kappa = \left(\frac{\sigma H_C}{\rho \Omega^2 R_C^4} \right)^{1/3}$$

mass transfer $$K_L = c_1 \frac{D}{H_C} \sqrt{\frac{Pe}{\kappa}}$$

comparison



A&R Figure 15
Flowrate (cm3/s)
80
60
40
scaling
Average mass transfer coefficient KLAV(m/s)*104
12.0
10.0
8.0
6.0
4.0
2.0
0.0
0
10
20
30
40
50
60
70
80
90
Rotational speed (rad/s)

detailed model objectives

- predict wave dynamics
  - amplitude, wavelength, velocity, frequency, shape
- predict mixing characteristics
  - residence time distribution
- predict heat transfer performance
  - effect of waves
- predict mass transfer performance
  - effect of waves
- model reactions
  - % conversion, selectivity

hydrodynamics

- parameters and scaling
- parabolised equations
- integral method
- nonlinear travelling waves
- full transient solution

variables

- film thickness

$$\tilde{h} = H_0 h \qquad H_0 = \sqrt{\nu / \Omega}$$

- coordinates

$$\tilde{t} = t / \Omega \qquad \tilde{r} = R_0 r \qquad \theta \qquad \tilde{z} = H_0 z \qquad R_0 = (Q_C / 2\pi)^{1/2} (\nu\Omega)^{-1/4}$$

- velocity components

$$\tilde{u}_r = \Omega R_0 u \qquad \tilde{u}_\theta = \Omega R_0 (r + v) \qquad \tilde{u}_z = \Omega H_0 w$$

- pressure

$$\tilde{p} = -\sigma \left[\frac{1}{\tilde{r}} \frac{\partial}{\partial \tilde{r}} \left(\tilde{r} \frac{\partial \tilde{h}}{\partial \tilde{r}} \right) \right]$$

dimensionless parameters

- film aspect ratio

$$\varepsilon_0^2 = \frac{H_0^2}{R_0^2} = \frac{2\pi}{Q_C}\sqrt{\frac{\nu^3}{\Omega}} << 1$$

neglected

- wave parameter

$$\lambda^2 = \frac{\sigma H_0}{\rho \Omega^2 R_0^4} = \frac{\sigma}{\rho}\left(\frac{2\pi}{Q_C}\right)^2\left(\frac{\nu}{\Omega}\right)^{3/2} << 1$$

retained

Navier–Stokes equations

parabolised and axisymmetric

$$\frac{1}{r}\frac{\partial(ru)}{\partial r}+\frac{\partial w}{\partial z}=0$$

$$\frac{\partial u}{\partial t}+u\frac{\partial u}{\partial r}+w\frac{\partial u}{\partial z}-\frac{(r+v)^2}{r}=\lambda^2\frac{\partial}{\partial r}\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial h}{\partial r}\right)\right]+\frac{\partial^2 u}{\partial z^2}$$

$$\frac{\partial v}{\partial t}+u\frac{\partial(r+v)}{\partial r}+\frac{u(v+r)}{r}+w\frac{\partial v}{\partial z}=\frac{\partial^2 v}{\partial z^2}$$

$$z=0 \qquad u=0 \qquad v=0 \qquad w=0$$

$$z=h(r,t) \qquad \frac{\partial u}{\partial z}=0 \qquad \frac{\partial v}{\partial z}=0 \qquad \frac{\partial h}{\partial t}+u\frac{\partial h}{\partial r}-w=0$$

integrated equations

$$\int_0^h \cdots dz \qquad f = r\int_0^h u\,dz \qquad g = r\int_0^h v\,dz$$

radial flow rate   angular momentum

$$\frac{\partial h}{\partial t} + \frac{1}{r}\frac{\partial f}{\partial r} = 0$$

$$\frac{\partial f}{\partial t} + \frac{\partial}{\partial r}\left(r\int_0^h u^2 dz\right) - \int_0^h v^2 dz = \lambda^2 h r \frac{\partial}{\partial r}\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial h}{\partial r}\right)\right] - r\left.\frac{\partial u}{\partial z}\right|_{z=0} + r^2 h + 2g$$

$$\frac{\partial g}{\partial t} + r\frac{\partial}{\partial r}\left(\int_0^h uv\,dz\right) + 2\int_0^h uv\,dz = -r\left.\frac{\partial v}{\partial z}\right|_{z=0} - 2f$$

approximated velocity profiles

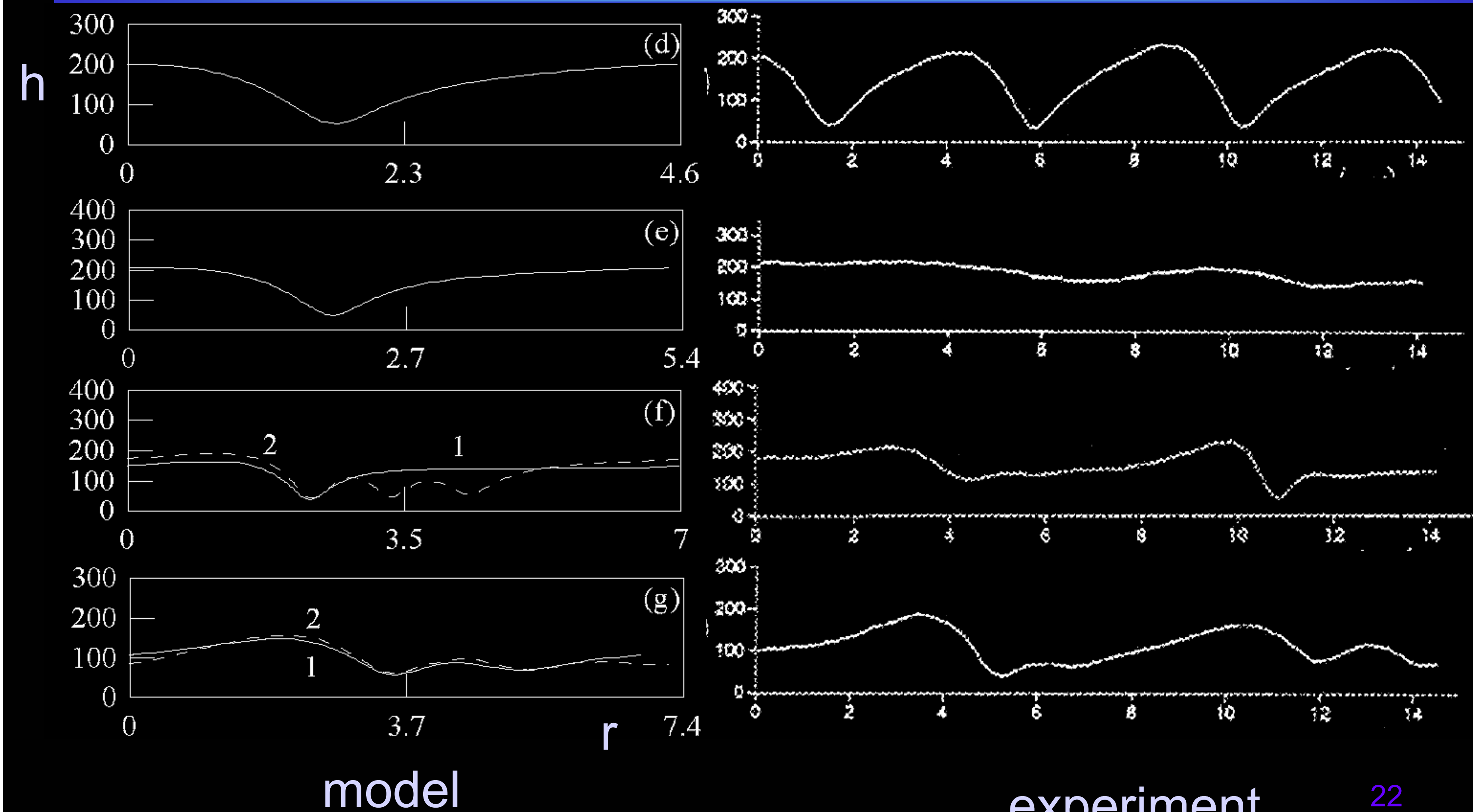
$$u = \frac{3f}{rh}(\zeta - \tfrac{1}{2}\zeta^2) = \frac{f}{rh}u_{(\zeta)} \qquad v = \frac{5g}{4rh}(2\zeta - \zeta^3 + \tfrac{1}{4}\zeta^4) = \frac{g}{rh}v_{(\zeta)}$$

$$\frac{\partial h}{\partial t} + \frac{1}{r}\frac{\partial f}{\partial r} = 0$$

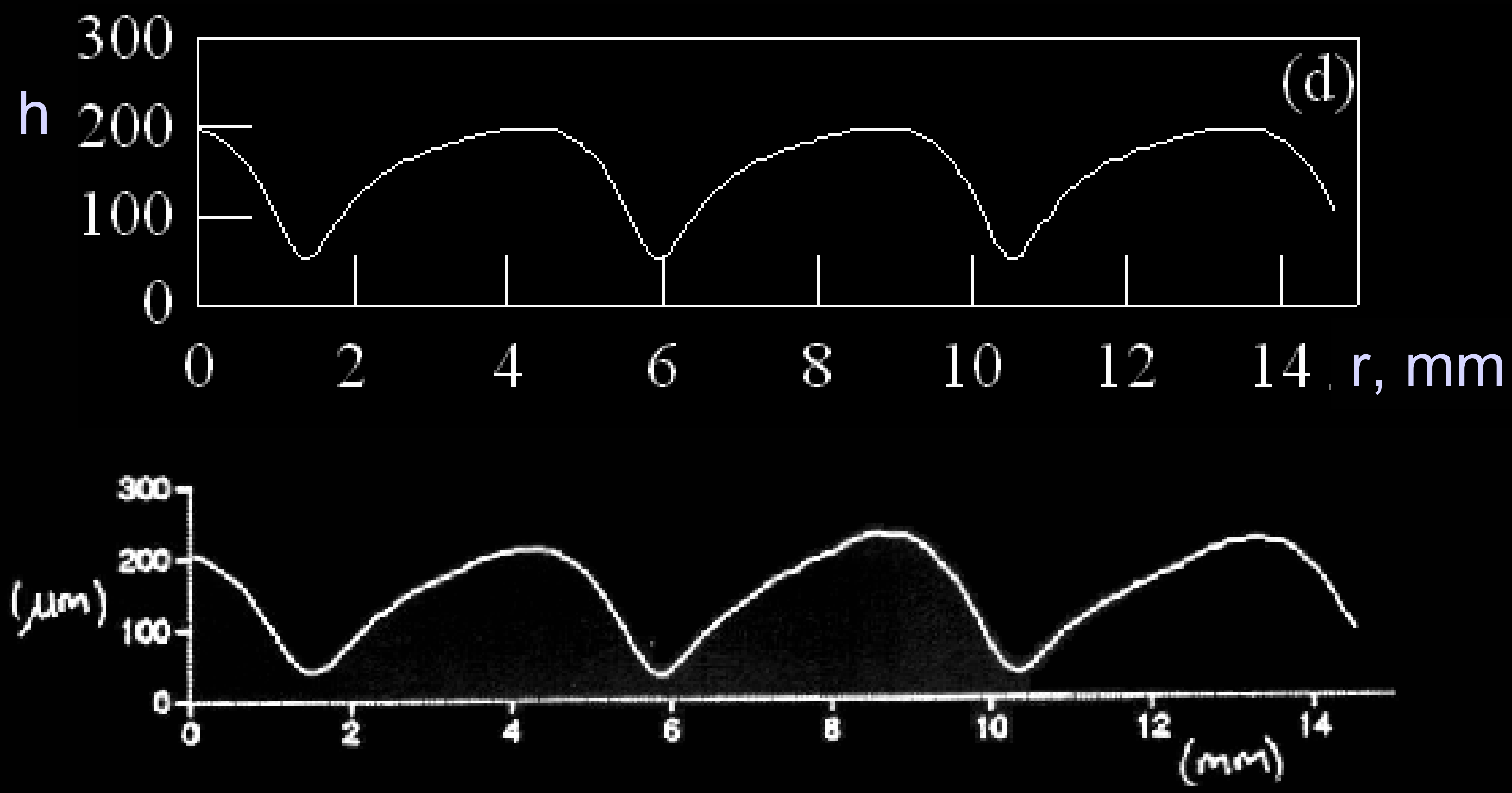
$$\frac{\partial f}{\partial t} + \frac{6}{5}\frac{\partial}{\partial r}\left[\frac{f^2}{rh}\right] - \frac{155}{126}\frac{g^2}{r^2 h} = \lambda^2 h r \frac{\partial}{\partial r}\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial h}{\partial r}\right)\right] - 3\frac{f}{h^2} + r^2 h + 2g$$

$$\frac{\partial g}{\partial t} + \frac{17}{14}\frac{1}{r}\frac{\partial}{\partial r}\left(\frac{fg}{h}\right) = -\frac{5}{2}\frac{g}{h^2} - 2f$$

nonlinear travelling waves
(localised)



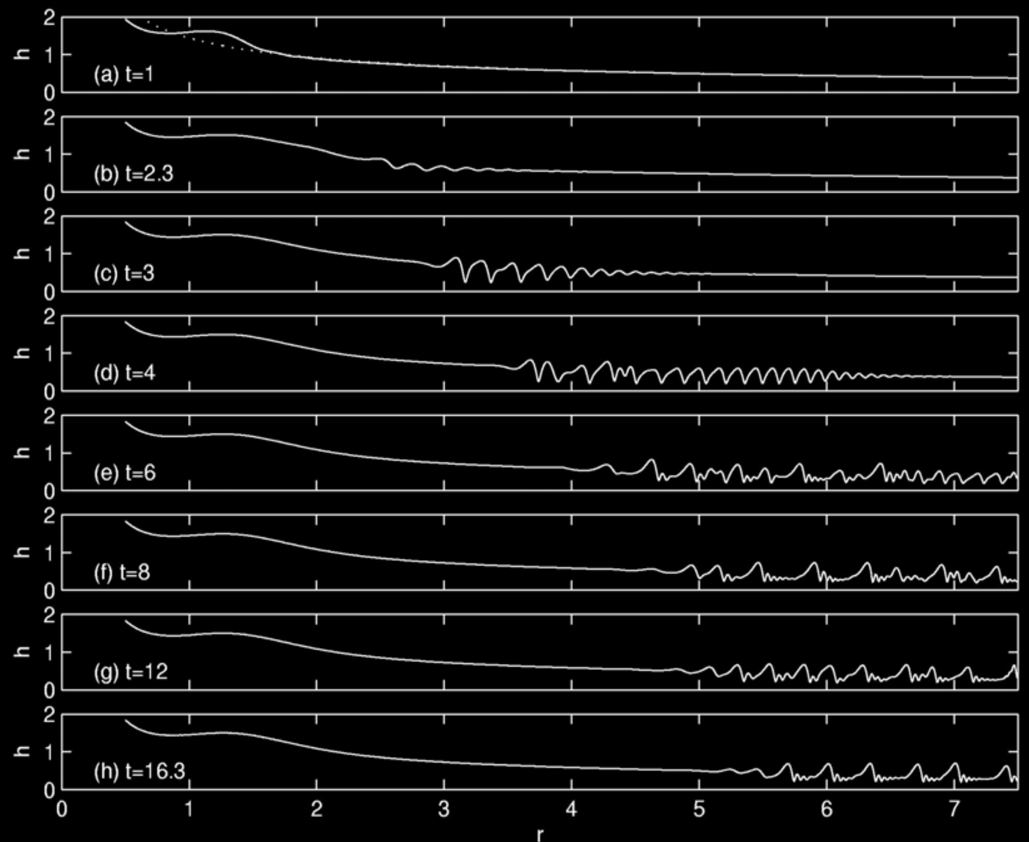
nonlinear travelling waves
(localised)



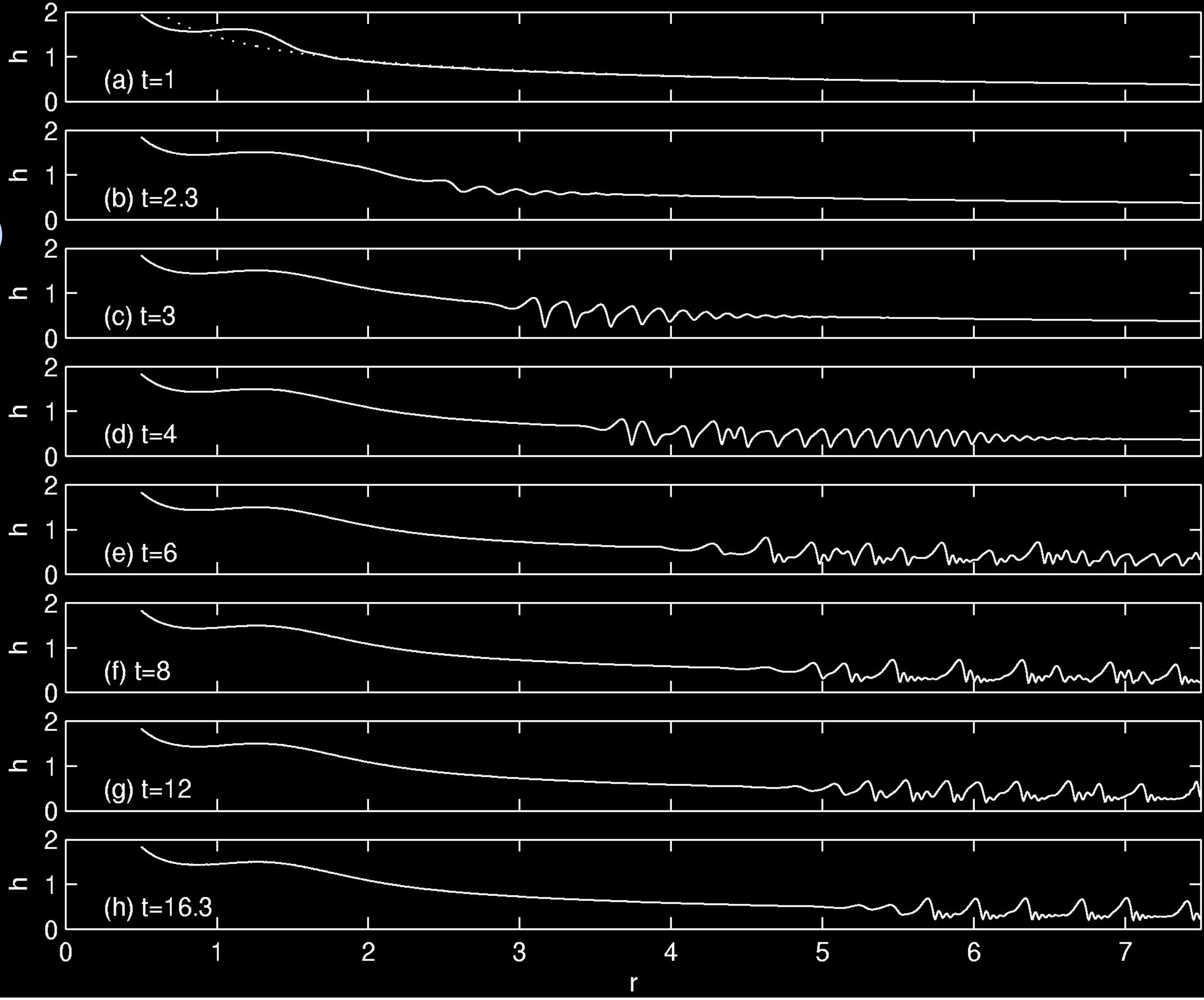
comparison of model (top) with experiment (bottom).

full transient solution

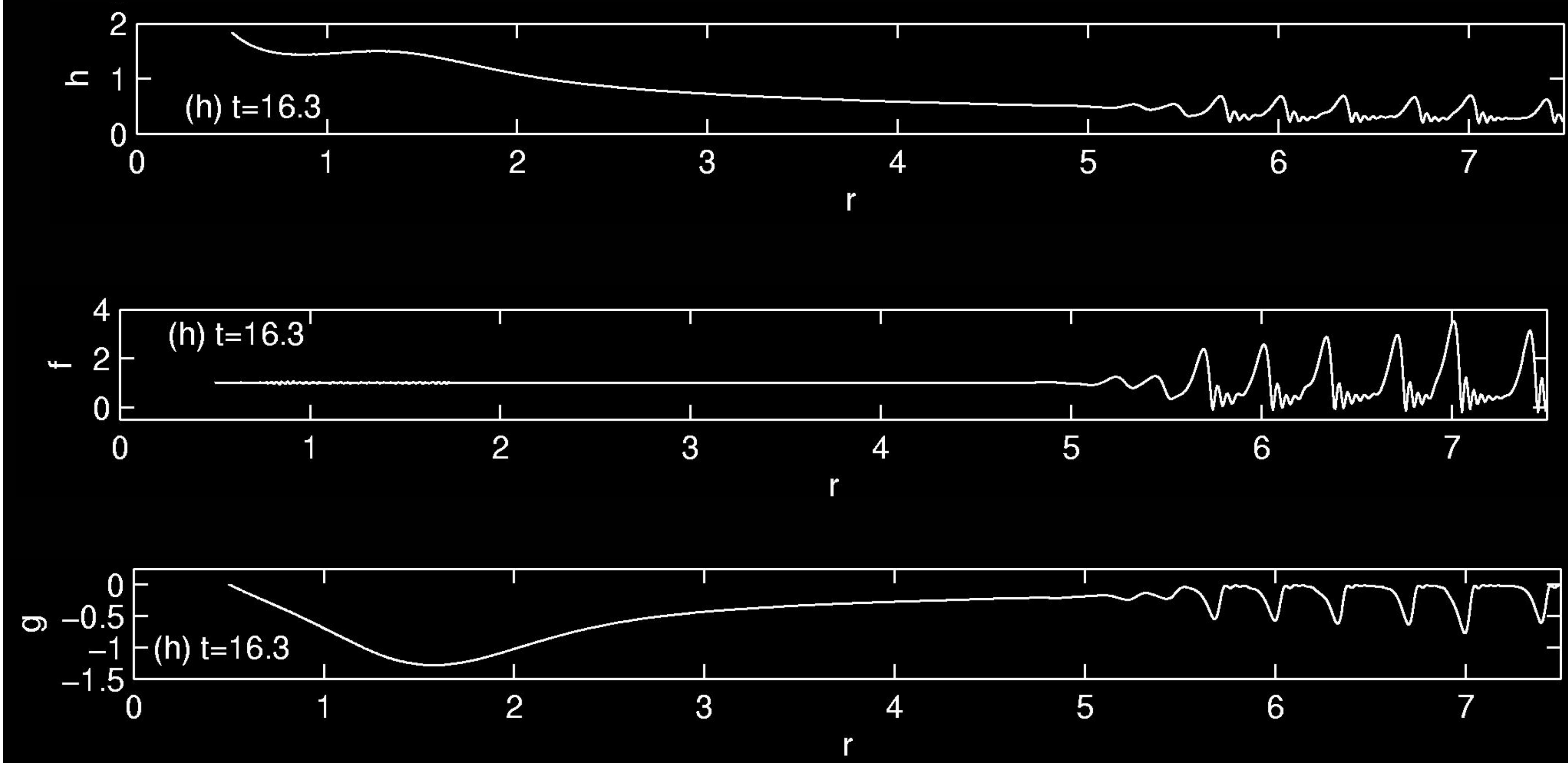
h(r,t)



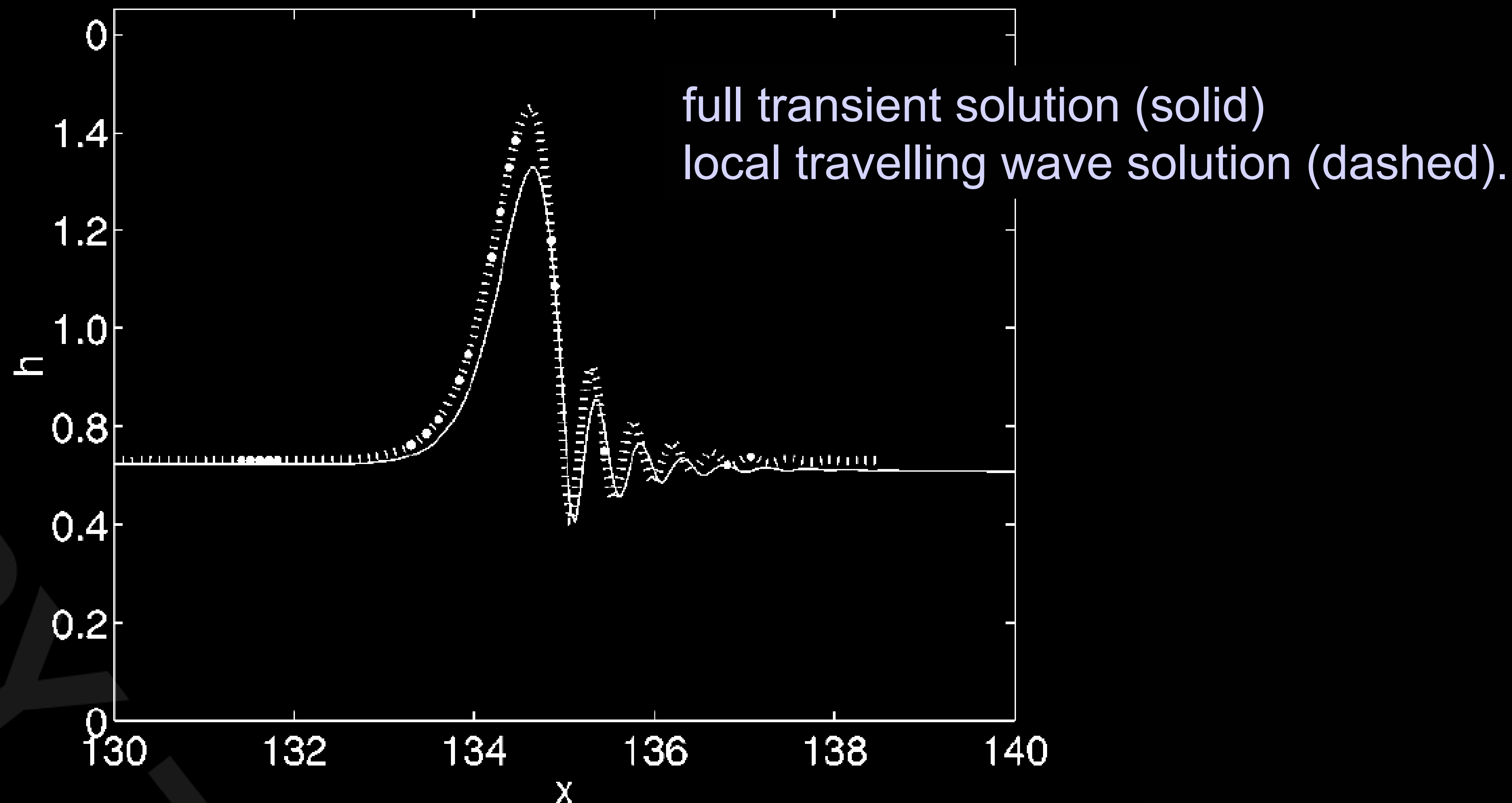
h(r,t)



full transient solution



nonlinear travelling wave



diffusion (mass transfer)

- parameters and scaling
- equations
- 2D solutions
- integral method
- asymptotic solution

parameters

oxygen uptake into a water film

- operating parameters
  - C_0 inlet concentration (0.2 ppm)
  - C_1 equilibrium (surface) concentration (9 ppm)
- fluid properties
  - D solute diffusion coefficient (10^{-9} m^2/s)

variables

- solute concentration

$$\tilde{C} = C_0 + (C_1 - C_0)C$$

- solute flux

$$\tilde{j} = D(\partial\tilde{C} / \partial\tilde{z})_{\tilde{z}=\tilde{h}}$$

- local mass transfer coefficient

$$\tilde{j} = K_L(C_1 - \overline{C})$$

- average (overall) mass transfer coefficient

$$\int_{\tilde{s}=0}^{\tilde{s}=\tilde{r}} \tilde{j}\, 2\pi\tilde{s}\, d\tilde{s} = \pi\tilde{r}^2 K_{AV}(C_1 - C_0)$$

dimensionless parameters

- Schmidt number

$$Sc^{-1} = \frac{D}{\nu} << 1$$

- Sherwood number

$$Sh_L(r) = \frac{K_L \tilde{h}}{D} = \frac{h}{(1-\phi)} \left(\frac{\partial C}{\partial z} \right)_{z=h}$$

$$Sh_{AV}(r) = \frac{K_{AV} H_0}{D} = \frac{2}{r^2} \left[\int_{s=0}^{s=r} \left(\frac{\partial C}{\partial z} \right)_{z=h} sds \right]$$

Diffusion equation
parabolised and axisymmetric

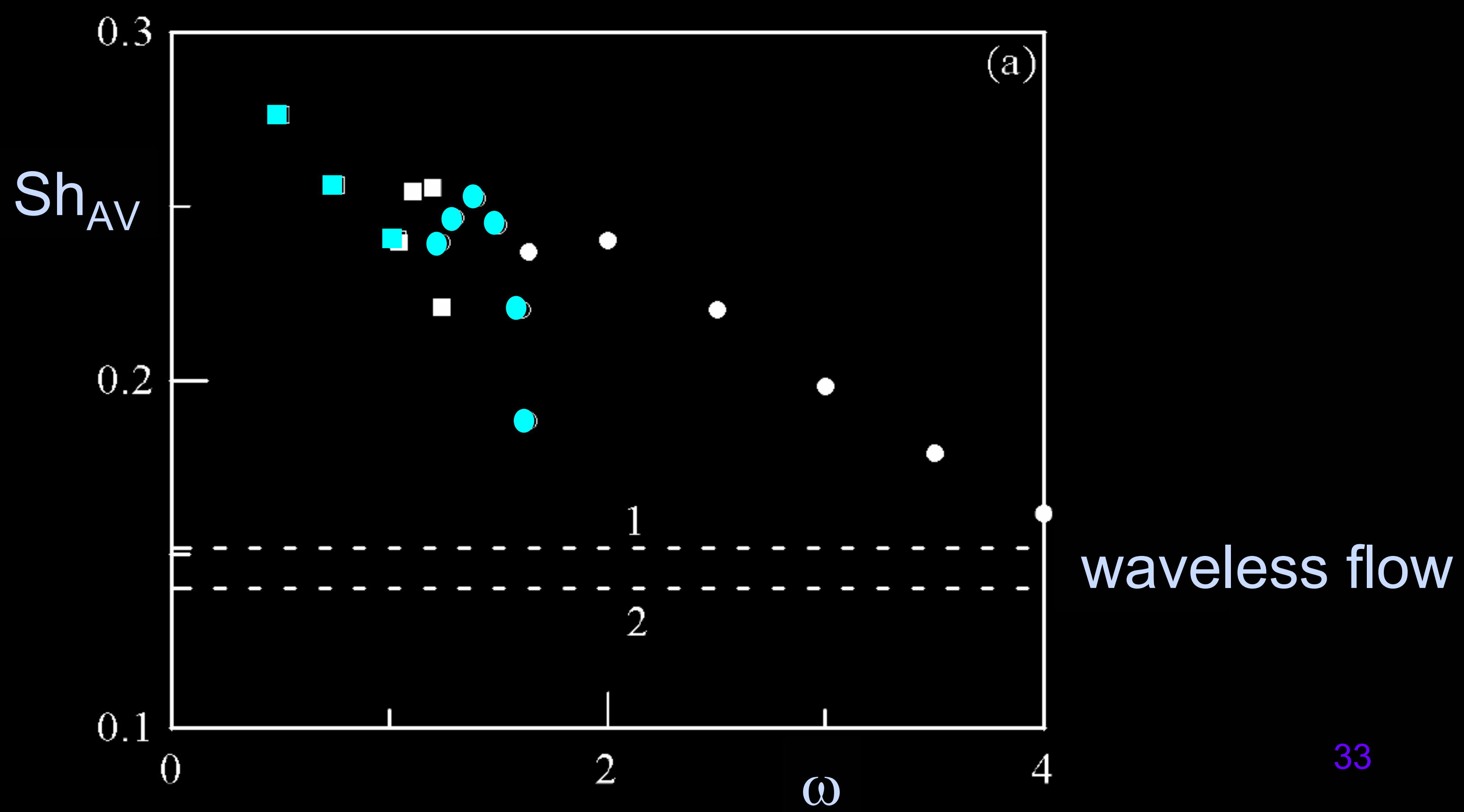
$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial r} + w\frac{\partial C}{\partial z} = Sc^{-1}\frac{\partial^2 C}{\partial z^2}$$

$$z = 0 \qquad \frac{\partial C}{\partial z} = 0$$

$$z = h(r,t) \qquad C = 1$$

2D numerical solution

- mass transfer enhancement by travelling waves



integrated equation

$$\frac{\partial \phi}{\partial t} = \frac{1}{h}\left[Sc^{-1}\frac{c_2}{h} + (c_1 - \phi)\frac{\partial h}{\partial t} - \frac{f}{r}\frac{\partial c_1}{\partial r} \right]$$

$$\phi = \frac{1}{h}\int_0^h C\,dz$$ mean concentration

$$c_1 = \frac{r}{f}\int_0^h uC\,dz$$ convective solute flux

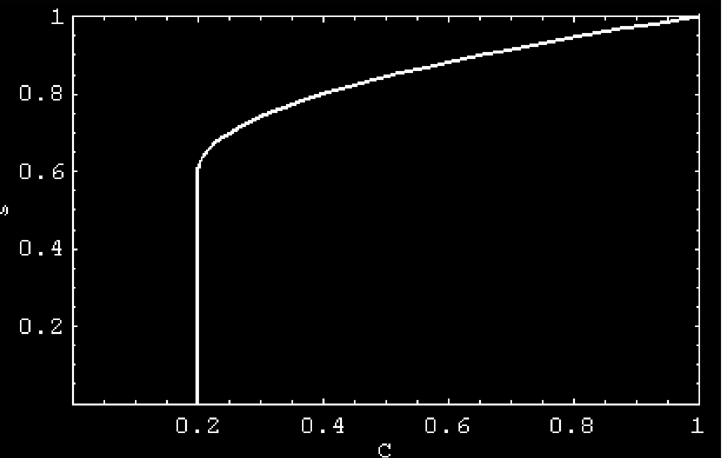
$$c_2 = h\left[\frac{\partial C}{\partial z}\right]_h$$ surface flux

approximated concentration profile

$$C = C_B + (1 - C_B)\left(1 - \frac{1-\zeta}{\beta}\right)^2 \qquad 1-\beta < \zeta < 1$$

$$C = C_B \qquad 0 < \zeta < 1-\beta$$

$\zeta = z/h_\omega$



- two variables

  C_B base concentration

  $\beta = \varpi^{1/2}$ boundary layer thickness

integrated equation

$$6\left(\frac{\sqrt{\varpi}-\frac{1}{3}\varpi}{1-C_B}\right)\left[\frac{\partial C_B}{\partial t}+\overline{u}\left(\frac{1-\frac{1}{2}\sqrt{\varpi}+\frac{1}{20}\varpi^{3/2}}{1-\frac{1}{3}\sqrt{\varpi}}\right)\frac{\partial C_B}{\partial r}\right]+\left[\frac{\partial \varpi}{\partial t}+u_s(1-\tfrac{3}{10}\varpi)\frac{\partial \varpi}{\partial r}\right]$$

$$=\frac{12Sc^{-1}}{h^2}+\varpi(1-\tfrac{3}{10}\varpi)\frac{1}{h}\frac{\partial h}{\partial t}$$

- one equation for two variables

$$6\left(\frac{\sqrt{\varpi}-\frac{1}{3}\varpi}{1-C_B}\right)\frac{DC_B}{Dt}+\frac{D\varpi}{Dt}=\Theta$$

partitioned equation

- if $\varpi < 1$ <u>or</u> $\Theta < 0$

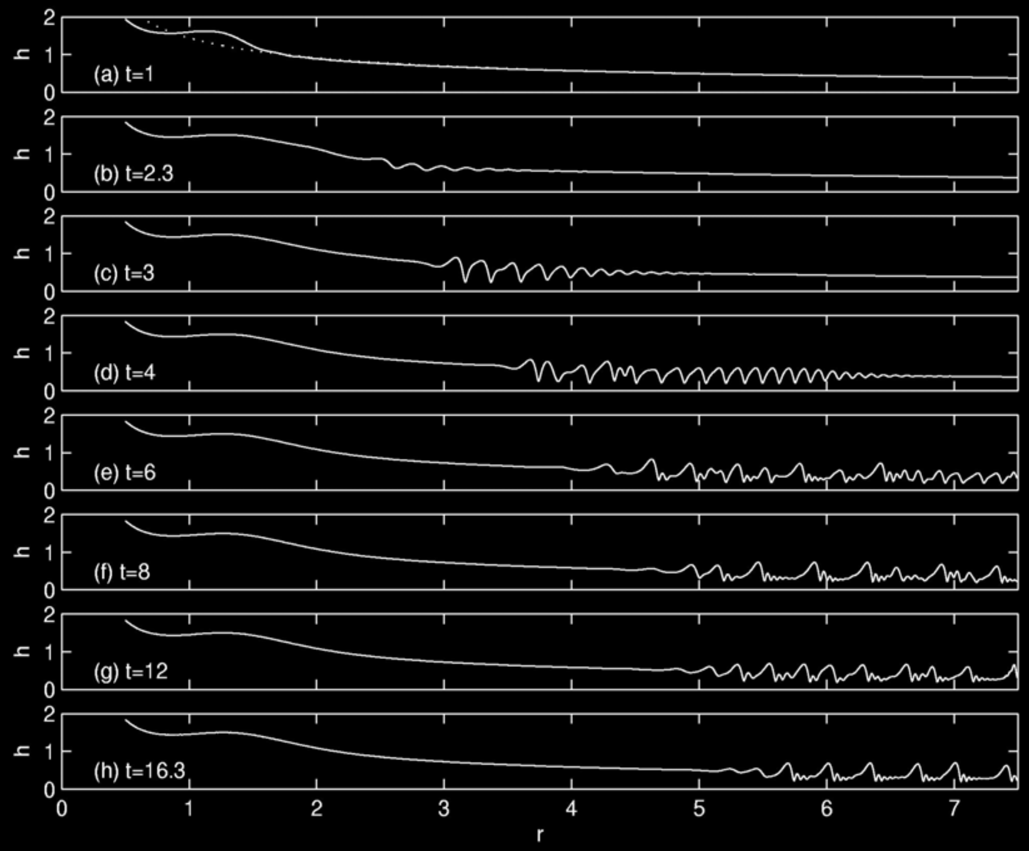
$$\frac{D\varpi}{Dt} = \Theta \qquad \frac{DC_B}{Dt} = 0$$

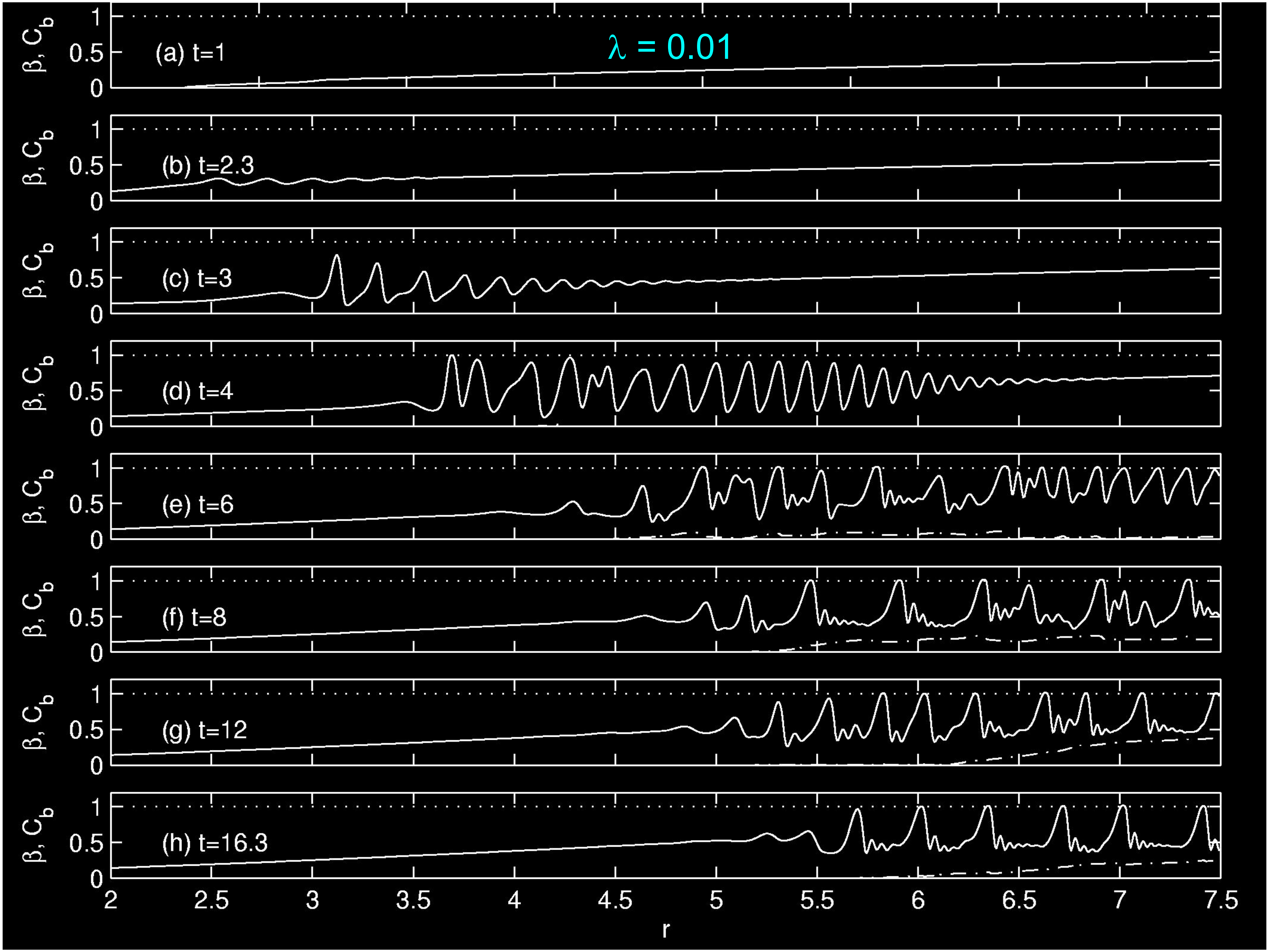
- if $\varpi = 1$ <u>and</u> $\Theta > 0$

$$\frac{D\varpi}{Dt} = 0 \qquad \frac{DC_B}{Dt} = \tfrac{1}{4}\Theta\left(1 - C_B\right)$$

full transient solution

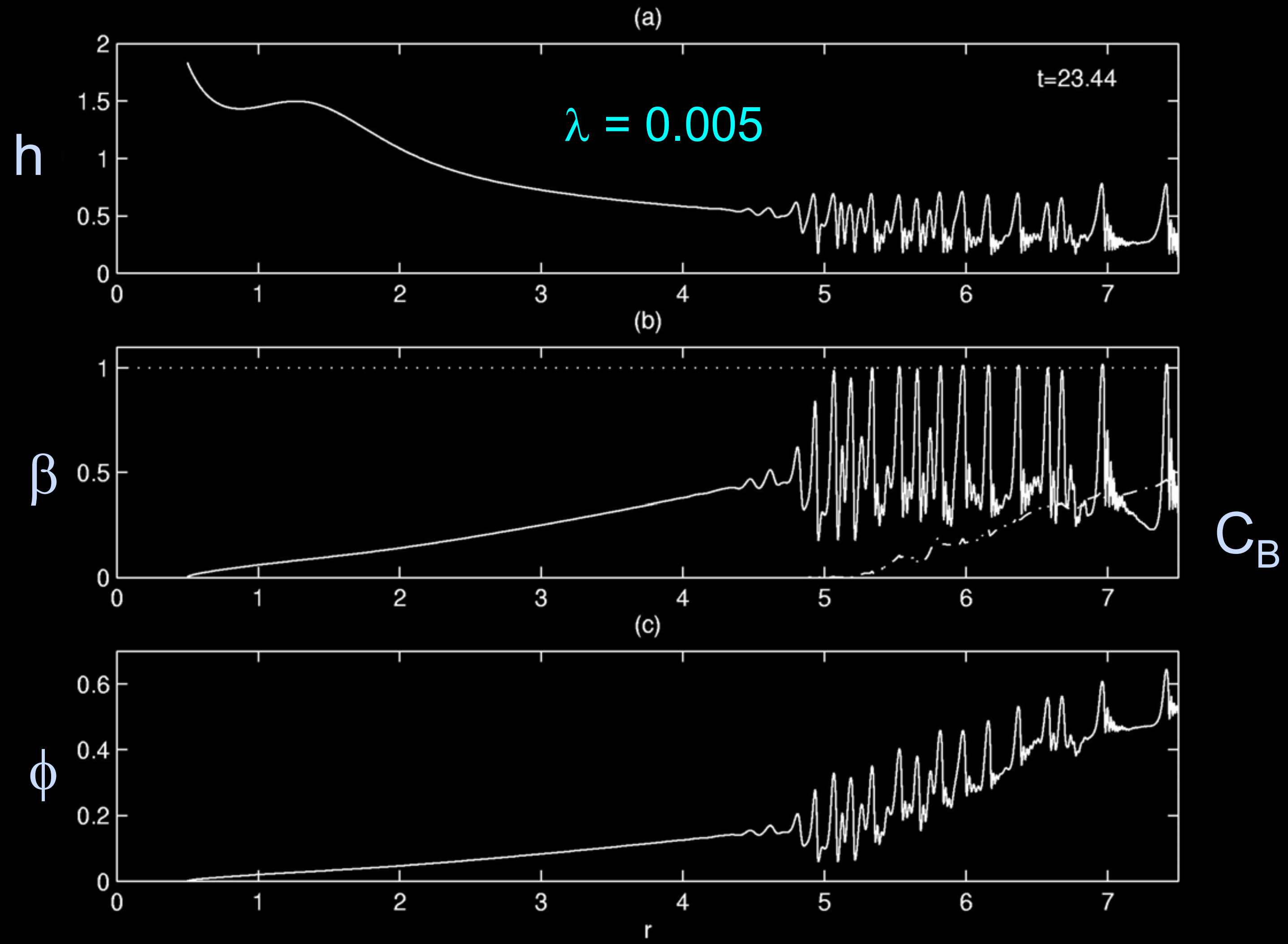
h(r,t)





λ = 0.01
(a) t=1
(b) t=2.3
(c) t=3
(d) t=4
(e) t=6
(f) t=8
(g) t=12
(h) t=16.3
β, C_b
r

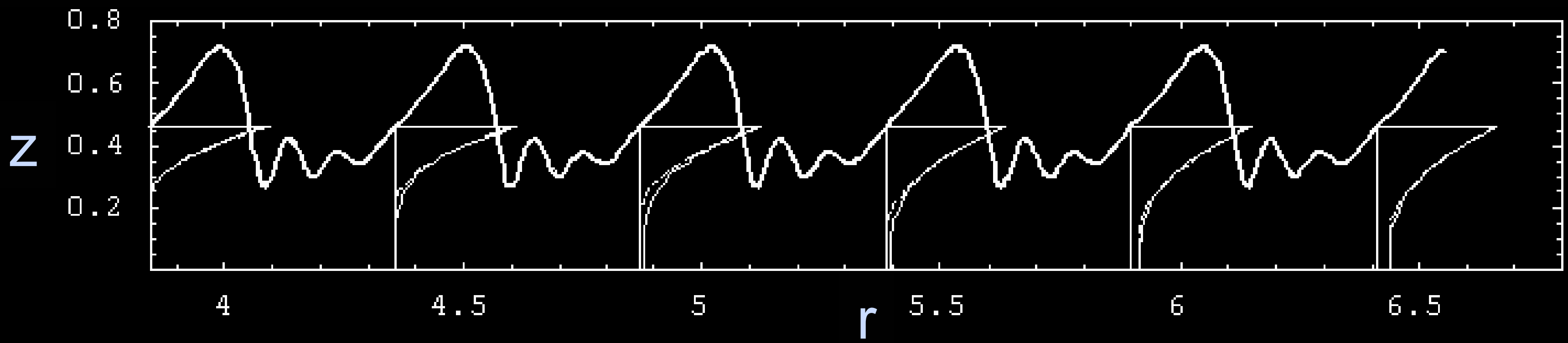
effect of λ

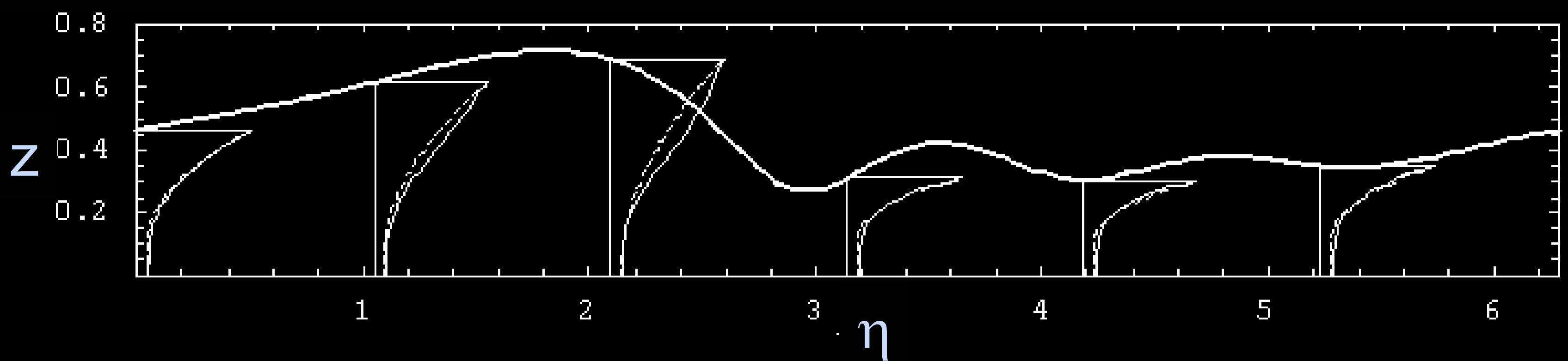


comparison

C(r,z,t)

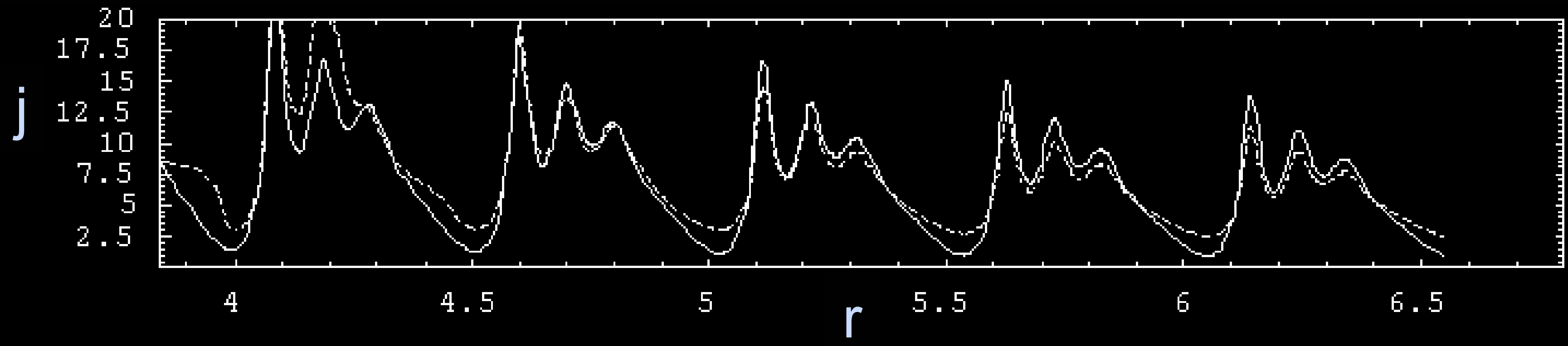
integral method (dashed)
2D numerical solution (solid)

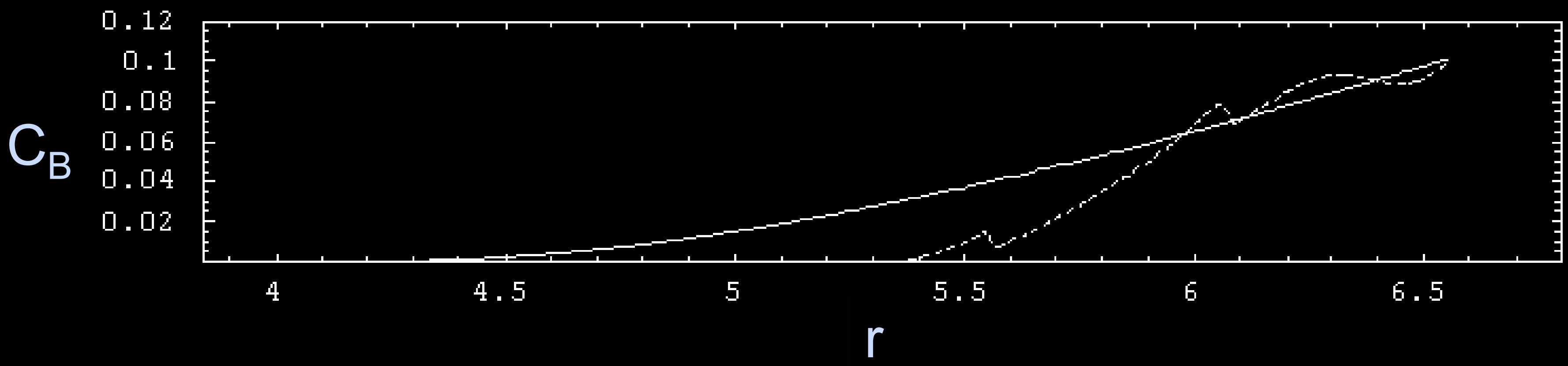




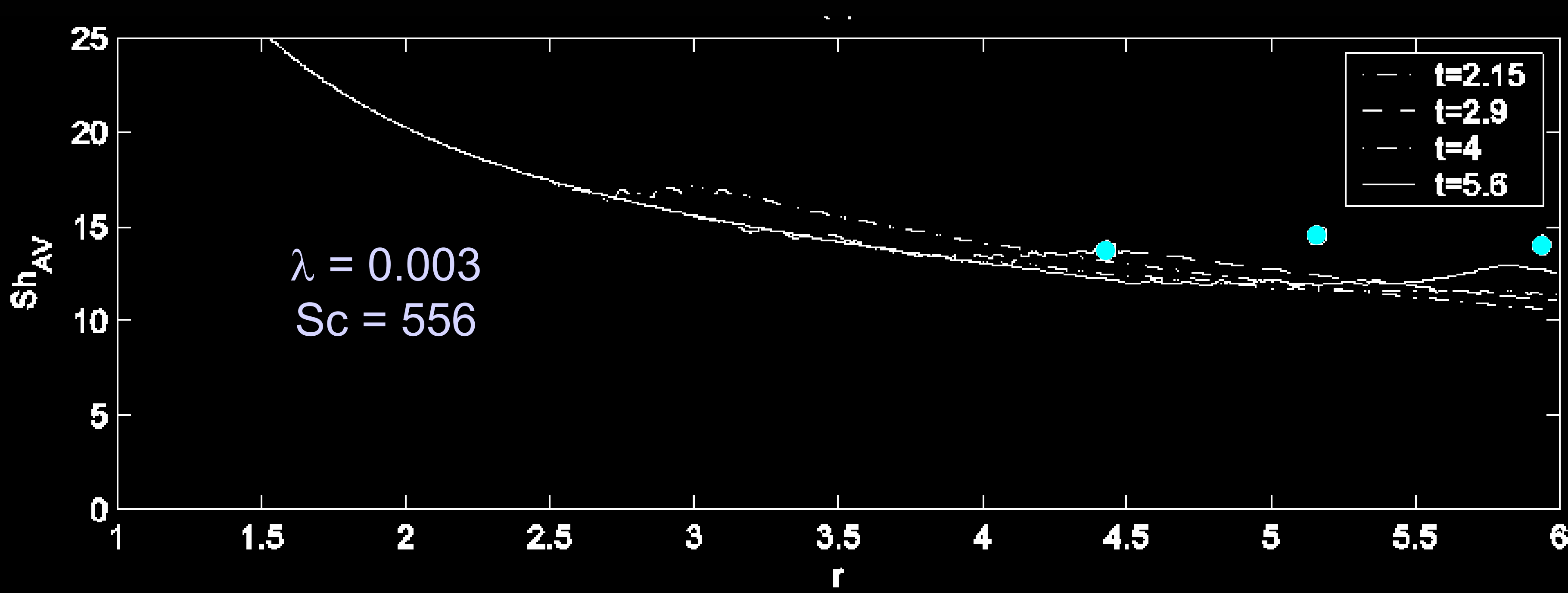
comparison

integral method (dashed)
2D solution (solid)

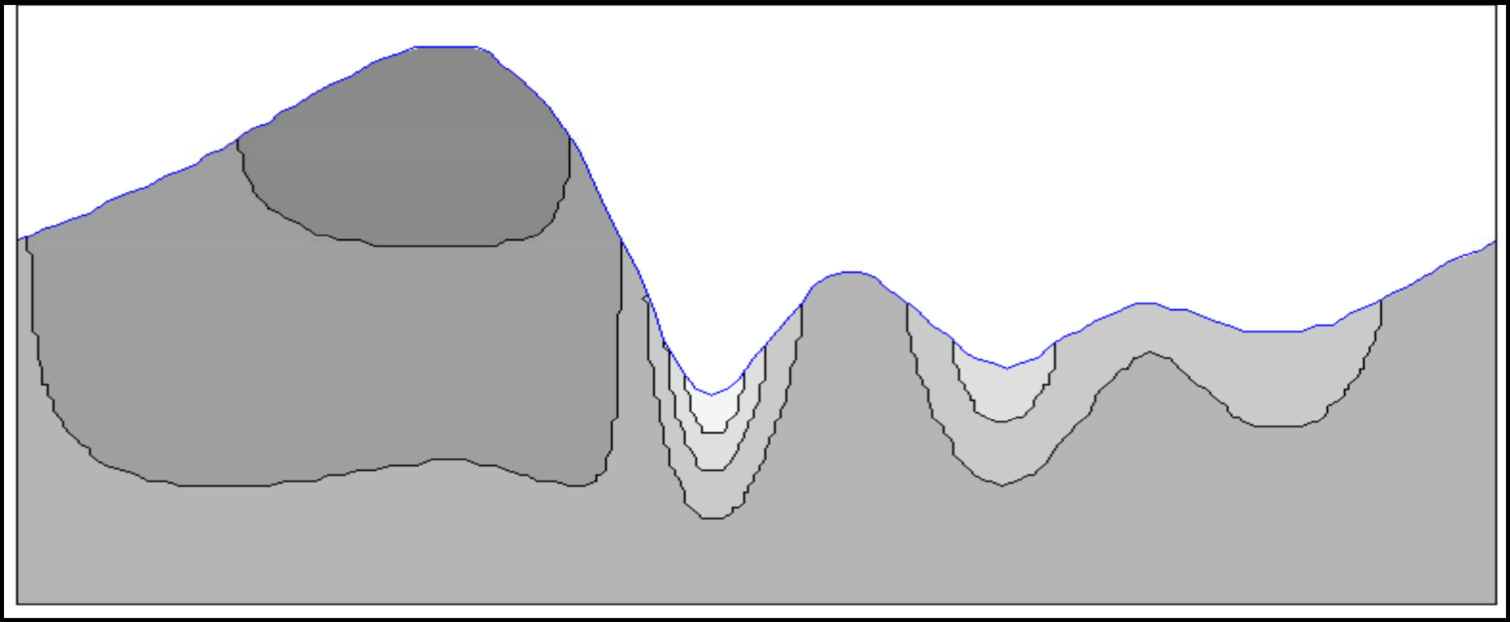


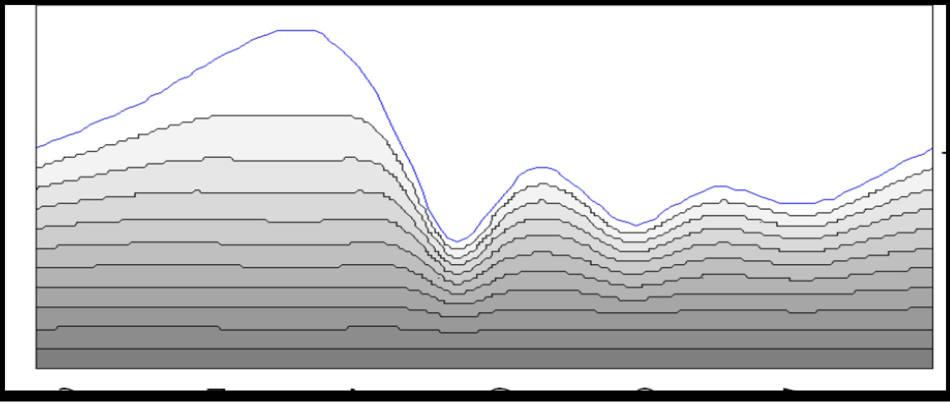


experimental data



apparent diffusion coefficient





summary

- hydrodynamics

$$\varepsilon_0^2 = \frac{H_0^2}{R_0^2} = \frac{2\pi}{Q_C}\sqrt{\frac{\nu^3}{\Omega}} << 1 \qquad \text{neglected}$$

$$\lambda^2 = \frac{\sigma H_0}{\rho \Omega^2 R_0^4} = \frac{\sigma}{\rho}\left(\frac{2\pi}{Q_C}\right)^2 \left(\frac{\nu}{\Omega}\right)^{3/2} << 1 \qquad \text{retained}$$

- integral method
- families of local travelling wave solutions
- full transient solutions
- comparison with experiments

summary

- diffusion

$$Sc^{-1} = \frac{D}{\nu} << 1$$

  - 2D numerical solution for travelling waves
  - integral method
  - single equation for two variables C_B and β
  - partitioned using 2^{nd} law
  - full transient solution
  - comparison with experiments

conclusions

- detailed model
  - sheds light on basic mechanisms
  - gives confidence in scaling results
- integral method
  - works pretty well
  - captures main features of concentration profile and solute flux
  - partitioning of equation seems OK
  - comparison with experiments is good