

Evaluation of Weighted Residual Methods for the Solution of the Chemical Reactor Pellet Model Equations

J. Solsvik, S. Tangen and H.A. Jakobsen
Department of Chemical Engineering
Norwegian University of Science and Technology (NTNU)
Trondheim, Norway

Abstract

Techniques in the family of weighted residual methods; the orthogonal collocation, Galerkin, tau, and least-squares methods, are adopted to solve a non-linear and highly coupled pellet problem. Based on a residual measure and problem matrix condition numbers, the Galerkin and tau methods are favorable solution techniques for the pellet equations. On the other hand, the orthogonal collocation is associated with less theoretical complexities and the simplest implementation. The accuracy of the orthogonal collocation method is similar to the least-squares method but with smaller condition numbers.

Keywords: pellet equations, weighted residual methods, orthogonal collocation, tau, Galerkin, least-squares.

1 Introduction

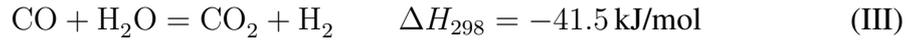
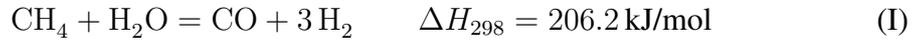
Heterogeneous catalysis is of outermost significance in many fields of gas conversion and processing in chemical industries. In this study, the orthogonal collocation, Galerkin, tau and least-squares methods are adopted solving a complex pellet model in the spectral framework. The evaluation of the techniques in the family of the weighted residual methods is based on convergence plots, problem matrix condition number, and implementation issues. The SMR process and the methanol synthesis are adopted for this investigation because the two processes cover various aspects of a chemical reaction, in particular, one of them is strongly diffusion limited, while the other is not.

During the last decade, the least-squares method has gained increasing interest in the chemical engineering field and is considered as a good candidate for solving reactor modeling problems. The least-squares method has been adopted for population balance problems, pseudo-homogeneous fixed bed reactor, and pellet problems

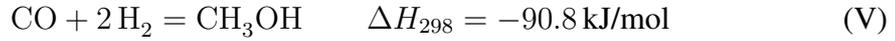
[1, 2, 3, 4, 5, 6, 7, 8]. Because the least-squares method is associated with the most complicated linear algebra theory and thus complicated implementation issues, it is of interest to investigate the performance of the least-squares technique relative to the more frequently used Galerkin, tau and orthogonal collocation methods solving the important pellet equations.

2 Chemical reactions

The steam methane reforming (SMR) process and the methanol synthesis are two important processes considered by the Norwegian gas industry for utilization of natural gas. In the present study the reaction kinetic model of the reforming and shift reactions (I)–(III) by Froment et al. [9] is adopted.



The kinetics of the methanol synthesis presented by Graaf et al. [11, 10] is used in this work and is based on the hydrogenation of CO_2 and CO as provided by reactions (IV) and (V), and the water–gas-shift reaction (III).



3 Mathematical modeling of porous catalyst pellets

A spherical geometry is adopted for the pellet and possible structural changes within the porous material are not considered. Moreover, symmetry is assumed in the sphere which results in one independent spatial variable in the radial dimension.

3.1 Pellet model equations

The continuity equation on mass basis is given as:

$$\frac{1}{r^2} \frac{\partial}{\partial r} (r^2 v^s \rho) = 0 \quad (1)$$

Species balance for components $i = 1, 2, \dots, n - 1$:

$$\frac{1}{r^2} \frac{\partial}{\partial r} (r^2 v^s \rho \omega_i) = -\frac{1}{r^2} \frac{\partial}{\partial r} (r^2 j_i^e) + \tilde{S}_i \quad (2)$$

By manipulation with the continuity equation (1) the species balance (2) can be written as:

$$v^s \rho \frac{\partial \omega_i}{\partial r} = -\frac{1}{r^2} \frac{\partial}{\partial r} (r^2 j_i^e) + \tilde{S}_i \quad (3)$$

Hence, the continuity is enforced in the species balances. The species balance for component $i = n$ is given by the summation formula:

$$\sum_{i=1}^n \omega_i = 1 \quad (4)$$

The multicomponent mass diffusion fluxes, j_i^e for components $i = 1, 2, \dots, n - 1$, are described by the Maxwell–Stefan closure [12]:

$$j_i^e = \frac{-\rho \omega_i \frac{\partial \ln(M)}{\partial r} - \rho \frac{\partial \omega_i}{\partial r} + M \omega_i \sum_{\substack{j=1 \\ j \neq i}}^n \frac{j_j^e}{M_j D_{ij}^e}}{M \sum_{\substack{j=1 \\ j \neq i}}^n \frac{\omega_j}{M_j D_{ij}^e}} \quad (5)$$

Moreover, the mass diffusion flux of Species $i = n$ is obtained from the summation relation:

$$\sum_{i=1}^n j_i^e = 0 \quad (6)$$

The heat balances are given as:

$$\rho C_{p_g} v^s \frac{\partial T}{\partial r} + \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 Q^e) = S \quad (7)$$

where the heat flux is given by Fourier's law:

$$Q^e = -\lambda^e \frac{\partial T}{\partial r} \quad (8)$$

The Darcy's law represents a relation between the pressure gradient and the viscous flow velocity:

$$v = -\frac{B}{\mu} \frac{\partial p}{\partial r} \quad \text{with} \quad B = \frac{d_{\text{pore}}^2}{32} \quad (9)$$

where the interstitial and superficial velocities are related by:

$$v^s = \epsilon v \quad (10)$$

The ideal gas law is used to give the density of the gas mixture:

$$p = \frac{\rho R T}{M} \quad (11)$$

The mass and heat source terms are given by, respectively:

$$\tilde{S}_i = (1 - \epsilon) M_i \rho_p r_i \quad (12)$$

$$S = (1 - \epsilon) \rho_p \sum (-\Delta H_{r_k}) r_k \quad (13)$$

3.2 Boundary conditions

The Dirichlet boundary conditions specified at the pellet surface are presented by:

$$\omega_i = \omega_{i,b} \quad (14)$$

$$T = T_b \quad (15)$$

$$p = p_b \quad (16)$$

At the symmetry point of the pellet, fluxes and velocities are assumed zero:

$$v = 0 \quad (17)$$

$$j_i^e = 0 \quad (18)$$

$$Q^e = 0 \quad (19)$$

4 Weighted residual methods

Given a one-dimensional problem in the following abstract formulation:

$$\mathcal{L}f(x) = g(x) \quad \text{in } \Omega \quad (20)$$

$$\mathcal{B}f(x) = f_\Gamma(x) \quad \text{on } \Gamma \quad (21)$$

where $f(x)$ is the unknown function, \mathcal{L} is a linear operator, and \mathcal{B} denotes the boundary condition operator. The problem is defined in the domain Ω and the boundary conditions is applied on Γ . Moreover, the functions g and f_Γ are given.

Spectral methods are based on using a representation of the solution $f(x) \in \mathcal{X}(\Omega)$ throughout the domain Ω via a truncated series expansion:

$$f(x) \approx f^P(x) = \sum_{j=0}^P \alpha_j \varphi_j(x) \quad (22)$$

where $\varphi_j(x)$ is the basis or trial function which span the subspace $\mathcal{X}^s(\Omega) \subset \mathcal{X}(\Omega)$.

Nodal basis functions are commonly adopted for implementation of spectral methods due to the resulting simplicity of the method. The nodal basis functions are generally defined based upon the Lagrange polynomials which are associated with a set of nodal points. The Lagrange polynomial can be written in product form as:

$$\ell_j(x) = \prod_{i=0, i \neq j}^P \frac{x - x_i}{x_j - x_i} \quad (23)$$

The nodal solution series expansion in terms of Lagrange polynomials is thus given as:

$$f(x) \approx f^P(x) = \sum_{j=0}^P f_j \ell_j(x) \quad (24)$$

Hence, in the nodal basis approximation the basis coefficients are the solution function value at the nodal points, i.e., $\alpha_j = f_j$. When the truncated series expansion (24) is substituted into the problem defined by equations (20) and (21), a residual will exist. A number of techniques are developed within the weighted residual framework to minimize the residual in some sense over the domain. In the sequel, the minimization of the residual as performed in the orthogonal collocation, least-squares, Galerkin and tau methods are outlined.

4.1 Least squares method

The least-squares formulation [1] is based on the minimization of a norm-equivalent functional. This consists in finding the minimizer of the residual in a certain norm. The norm-equivalent functional is given by:

$$\begin{aligned} \mathcal{J}(f; g, f_\Gamma) &\equiv \frac{1}{2} \|\mathcal{L}f - g\|_{\mathcal{X}(\Omega)}^2 + \frac{1}{2} \|\mathcal{B}f - f_\Gamma\|_{\mathcal{X}(\Omega)}^2 \\ &= \frac{1}{2} \|\mathcal{R}_\Omega(f)\|_{\mathcal{X}(\Omega)}^2 + \frac{1}{2} \|\mathcal{R}_\Gamma(f)\|_{\mathcal{X}(\Omega)}^2 \end{aligned} \quad (25)$$

where the norms are defined like:

$$\|\bullet\|_{\mathcal{X}(\Omega)}^2 = \langle \bullet, \bullet \rangle_{\mathcal{X}(\Omega)} = \int_{\Omega} \bullet \bullet \, d\Omega \quad (26)$$

$$\|\bullet\|_{\mathcal{X}(\Gamma)}^2 = \langle \bullet, \bullet \rangle_{\mathcal{X}(\Gamma)} = \int_{\Gamma} \bullet \bullet \, d\Gamma \quad (27)$$

and the residuals are given as:

$$\mathcal{R}_\Omega(f) = \mathcal{L}f - g \quad \text{in } \Omega \quad (28)$$

$$\mathcal{R}_\Gamma(f) = \mathcal{B}f - f_\Gamma \quad \text{on } \Gamma \quad (29)$$

Based on variational analysis, the minimization statement is equivalent to: Find $f \in \mathcal{X}(\Omega)$ such that

$$\lim_{\epsilon \rightarrow 0} \frac{d\mathcal{J}(f + \epsilon v; g, f_\Gamma)}{d\epsilon} = 0 \quad \forall v \in \mathcal{X}(\Omega) \quad (30)$$

It follows that it is possible to write the necessary condition as: Find $f \in \mathcal{X}(\Omega)$ such that:

$$\langle \mathcal{L}f, \mathcal{L}v \rangle_{\mathcal{X}(\Omega)} + \langle \mathcal{B}f, \mathcal{B}v \rangle_{\mathcal{X}(\Gamma)} = \langle g, \mathcal{L}v \rangle_{\mathcal{X}(\Omega)} + \langle f_\Gamma, \mathcal{B}v \rangle_{\mathcal{X}(\Gamma)} \quad (31)$$

Inserting approximation (24) and choosing systematically

$$v = \ell_{j=0}(x), \ell_{j=1}(x), \dots, \ell_{j=P}(x) \quad (32)$$

the following algebraic system is achieved:

$$\mathcal{A}f = \mathbf{F} \quad (33)$$

where the matrix $\mathcal{A} \in \mathbb{R}^{(P+1) \times (P+1)}$ and vectors $\mathbf{F}, \mathbf{f} \in \mathbb{R}^{(P+1) \times 1}$ are defined as:

$$[\mathcal{A}]_{ij} = \langle \mathcal{L}l_j(x), \mathcal{L}l_i(x) \rangle_{\mathcal{X}(\Omega)} + \langle \mathcal{B}l_j(x), \mathcal{B}l_i(x) \rangle_{\mathcal{X}(\Gamma)} \quad (34)$$

$$[\mathbf{F}]_i = \langle g, \mathcal{L}l_i(x) \rangle_{\mathcal{X}(\Omega)} + \langle f_\Gamma, \mathcal{B}l_i(x) \rangle_{\mathcal{X}(\Gamma)} \quad (35)$$

$$[\mathbf{f}]_i = f_i = f(\mathbf{x}_i) \quad (36)$$

The inner products (34) and (35) are approximated by a quadrature rule:

$$[\mathcal{A}]_{ij} = \sum_{i_q=0}^P W_{i_q} \mathcal{L}l_j(\mathbf{x}_{i_q}) \mathcal{L}l_i(\mathbf{x}_{i_q}) + \sum_{i_q=0}^P W_{i_q} \mathcal{B}l_j(x_{i_q}) \mathcal{B}l_i(x_{i_q}) \quad (37)$$

$$[\mathbf{F}]_i = \sum_{i_q=0}^P W_{i_q} g(\mathbf{x}_{i_q}) \mathcal{L}l_i(\mathbf{x}_{i_q}) + \sum_{i_q=0}^P W_{i_q} f_\Gamma(\mathbf{x}_{i_q}) \mathcal{B}l_i(\mathbf{x}_{i_q}) \quad (38)$$

4.2 Galerkin and tau methods

There are two conceptually different options available for the formulation of the spectral solution methods, these are: (i) the variational methods and (ii) the weighted residual methods. In the sequent, the Galerkin, tau and orthogonal collocation methods are outlined based on the minimization of weighted integrals or inner products. Moreover, as opposite to the weak formulation in the least-squares method, the strong formulation is applied in the Galerkin, tau and orthogonal collocation methods. In this context, the weak formulation is associated with the residual minimization of both the governing equations and the boundary conditions, whereas in the strong formulation the residual of the governing equations is minimized in Ω and the boundary conditions are enforced to be fulfilled on Γ . Hence, the residual minimization statement of the Galerkin, tau and orthogonal collocation methods can be given by the following inner product:

$$\langle \psi_i, \mathcal{R}_\Omega^P \rangle = \int_\Omega \mathcal{R}_\Omega(x; f_0, f_1, \dots, f_j, \dots, f_P) \psi_i(x) \, d\Omega = 0 \quad \forall i = 0, 1, \dots, P \quad (39)$$

Each choice of the weighting function ψ correspond to a different residual estimate within the computational domain. In the Galerkin method, the residual is constrained to be orthogonal to each of the basis functions in the problem domain. Hence, the weighting function is identical to the basis function, i.e., in this study, $\psi_i(x) = l_i(x)$

for $i = 0, 1, \dots, P$. The inner product of the Ω -domain (39) may be given as:

$$\begin{aligned}
\langle \ell_i(x), \mathcal{R}_\Omega(x; f_0, f_1, \dots, f_j, \dots, f_P) \rangle &= \int_\Omega \mathcal{R}_\Omega(x; f_0, f_1, \dots, f_j, \dots, f_P) \ell_i(x) \, d\Omega \\
&= \sum_{j=0}^P f_j \int_\Omega [\ell_i(x) \mathcal{L} \ell_j(x) - \ell_i(x) g(x)] \, d\Omega \\
&= \sum_{j=0}^P f_j \sum_{i_q=0}^P [\ell_i(x_{i_q}) \mathcal{L} \ell_j(x_{i_q}) - \ell_i(x_{i_q}) g(x_{i_q})] W_{i_q} \\
&= 0 \quad \forall i = 0, 1, \dots, P
\end{aligned} \tag{40}$$

where the approximation (24), residual definition (28), and a quadrature rule are adopted. In the Galerkin method, it is required that each of the basis function exactly satisfy the boundary conditions, hence, some linear combinations of the polynomials that fulfill the boundary conditions must be performed. Thus, deliberately structuring the trial solution to satisfy the boundary conditions is a common practice in applying the Galerkin method. Given the boundary condition $f(x_{\min}) = f_\Gamma$, the algebraic equation system (33) of the Galerkin method is given as:

$$[\mathcal{A}]_{ij} = \sum_{i_q=0}^P \ell_i(x_{i_q}) \mathcal{L} \ell_j(x_{i_q}) W_{i_q} \quad \text{for } i = 1, \dots, P \quad \text{and } j = 1, \dots, P \tag{41}$$

$$[\mathbf{F}]_i = \sum_{i_q=0}^P \ell_i(x_{i_q}) g(x_{i_q}) W_{i_q} \quad \text{for } i = 1, \dots, P \tag{42}$$

$$[\mathcal{A}] = \begin{bmatrix} a_{1,1} & a_{1,2} & \dots & a_{1,P} \\ a_{2,1} & a_{2,2} & \dots & a_{2,P} \\ \vdots & \vdots & \ddots & \vdots \\ a_{P,1} & a_{P,2} & \dots & a_{P,P} \end{bmatrix} \tag{43}$$

$$[\mathbf{f}] = \begin{bmatrix} f_1 \\ f_2 \\ \vdots \\ f_P \end{bmatrix} \tag{44}$$

$$[\mathbf{F}] = \begin{bmatrix} F_1 - a_{1,0} f_\Gamma \\ F_2 - a_{2,0} f_\Gamma \\ \vdots \\ F_P - a_{P,0} f_\Gamma \end{bmatrix} \tag{45}$$

The tau method is similar to the Galerkin method. The essential difference between the Galerkin and the tau methods is that in the tau method, the trial functions are not required to satisfy the boundary conditions individually. Thus, the inner product of

the tau method may also be describe according to (40) but the treatment of the boundary conditions differ from the way boundary conditions are handled in the Galerkin method. In the tau method, the boundary conditions are enforced as additional equations and in order to get a system of equations where the number of unknowns is identical to the number of equations, the equation system has to be relaxed by n residual equations and replaced by the n boundary conditions. Hence, given the boundary condition $f(x_{\min}) = f_{\Gamma}$, the algebraic equation system (33) of the tau method is given as:

$$[\mathcal{A}]_{ij} = \sum_{i_q=0}^P \ell_i(x_{i_q}) \mathcal{L} \ell_j(x_{i_q}) W_{i_q} \quad \text{for } i = 1, \dots, P \quad \text{and } j = 0, 1, \dots, P \quad (46)$$

$$[\mathbf{F}]_i = \sum_{i_q=0}^P \ell_i(x_{i_q}) g(x_{i_q}) W_{i_q} \quad \text{for } i = 1, \dots, P \quad (47)$$

$$[\mathcal{A}] = \begin{bmatrix} 1 & 0 & \dots & 0 \\ a_{1,0} & a_{1,1} & \dots & a_{1,P} \\ a_{2,0} & a_{2,1} & \dots & a_{2,P} \\ \vdots & \vdots & \ddots & \vdots \\ a_{P,0} & a_{P,1} & \dots & a_{P,P} \end{bmatrix} \quad (48)$$

$$[\mathbf{f}] = \begin{bmatrix} f_0 \\ f_1 \\ \vdots \\ a_P \end{bmatrix} \quad (49)$$

$$[\mathbf{F}] = \begin{bmatrix} f_{\Gamma} \\ F_1 \\ \vdots \\ F_P \end{bmatrix} \quad (50)$$

4.3 Orthogonal collocation method

In the orthogonal collocation method, the weighting function ψ in Eq. (39) is the Dirac delta function, i.e., $\psi_i(x) = \delta(x - x_i)$. The property of the Dirac delta function implies the following equalities:

$$\int_{\Omega} \delta(x - x_i) dx = 1 \Big|_{x=x_i} \quad (51)$$

$$\int_{\Omega} \delta(x - x_i) dx = 0 \Big|_{x \neq x_i} \quad (52)$$

Accordingly, at the location of the node points the residual is forced to zero such that the differential equations are exactly satisfied at these points:

$$\int_{\Omega} \mathcal{R}(x; f_{P,0}, f_{P,1}, \dots, f_{P,P}) \delta(x - x_i) dx = \mathcal{R}(x; f_{P,0}, f_{P,1}, \dots, f_{P,P}) \Big|_{x=x_i} = 0 \quad (53)$$

The approximated solution of $f(x)$ by the collocation method is thus represented by finding a particular set of unknown coefficients $\{f_j, j = 0, 1, \dots, P\}$ which satisfy equations (53). The equation system (33) can be defined as:

$$[\mathcal{A}]_{ij} = \mathcal{L}l_j(x_i) \quad (54)$$

$$[\mathbf{F}]_i = g(x_i) \quad (55)$$

Moreover, the treatment of the boundary conditions in the orthogonal collocation method can follow both the framework of the tau and Galerkin methods.

5 Results and discussion

A steady model is derived describing the temperature variations, viscous flow velocity, pressure, mass and heat fluxes, gas density, and species concentrations within the voids and channels of a catalyst pellet. The pellet model is solved by the orthogonal collocation, Galerkin, tau and least-squares methods, which are techniques in the family of weighted residual methods. The reaction kinetics of both the SMR and methanol synthesis are adopted for the present analysis of the numerical methods. Adopting the reactor operating conditions as given in table 1, figures 1 (MeOH) and 2 (SMR) elucidate large concentration gradients within the SMR catalyst pellet compared to the less intra-particle mass transfer limited methanol synthesis.

Because the pellet problem is non-linear, linearization by the Picard method is adopted. To access the convergence of the model, the following convergence error measure is defined:

$$\|\text{Res}\| = \sqrt{\int_{\Omega} (\mathcal{A}f - \mathbf{F})^2 d\Omega} \quad (56)$$

The convergence plot of the methanol synthesis is presented in figure 3 for polynomial orders $P = N + 1$; $N = 10$, whereas the convergence plots of the SMR process is presented in figure 4 for polynomial orders $P = N + 1$; $N = 40$. Both the Galerkin and tau methods deviate minor in the residual measure with the number of iterations. Moreover, considering the solution accuracy, the Galerkin and tau methods are favorable to the orthogonal collocation and least-squares method, in particular for the larger gradient case, i.e. SMR process. The least-squares method obtains a significantly larger condition number than the remaining methods.

As the residual in the orthogonal collocation method is minimized at the collocation points, the implementation complexity and computational costs are in favor for this weighted residual method. Moreover, due to the linear manipulation of the boundary conditions the Galerkin appeared as the most time consuming method to implement.

Description	MeOH	SMR
d (m)	0.0042	0.0173
d_{pore} (nm)	40	40
ϵ (-)	0.5	0.528
τ (-)	4	3.5
p_b (bar)	80	29
T_b (K)	500	800
ρ_p (kg/m ³)	1775	2300
λ^e (W/m/K)	26	25
$\tilde{C}p_p$ (J/kg/K)	1000	1000
$x_{b,i}$ (-)		
MeOH	0.0022	-
CO	0.058	6.3581e-005
CO ₂	0.022	0.0080931
H ₂	0.89	0.025567
H ₂ O	0.0005	0.71335
CH ₄	0.0273	0.21218
N ₂	-	0.040755

Table 1: Specifications of the reactor operating conditions used in the simulations of the methanol synthesis and SMR process.

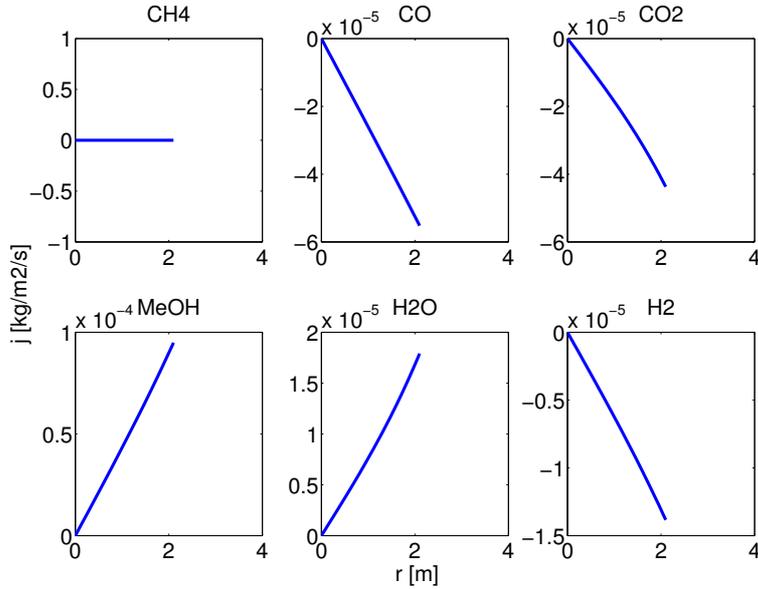


Figure 1: Simulation results: mass diffusion fluxes of the methanol synthesis.

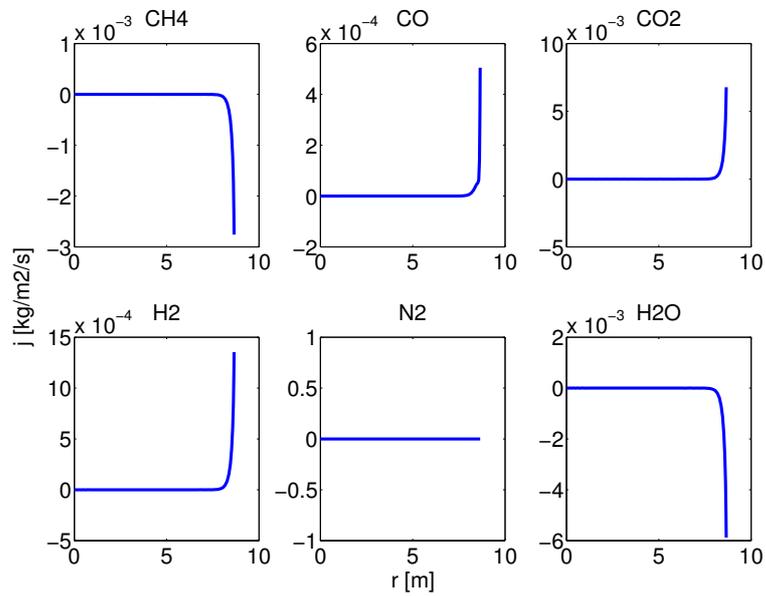


Figure 2: Simulation results: mass diffusion fluxes of the SMR process.

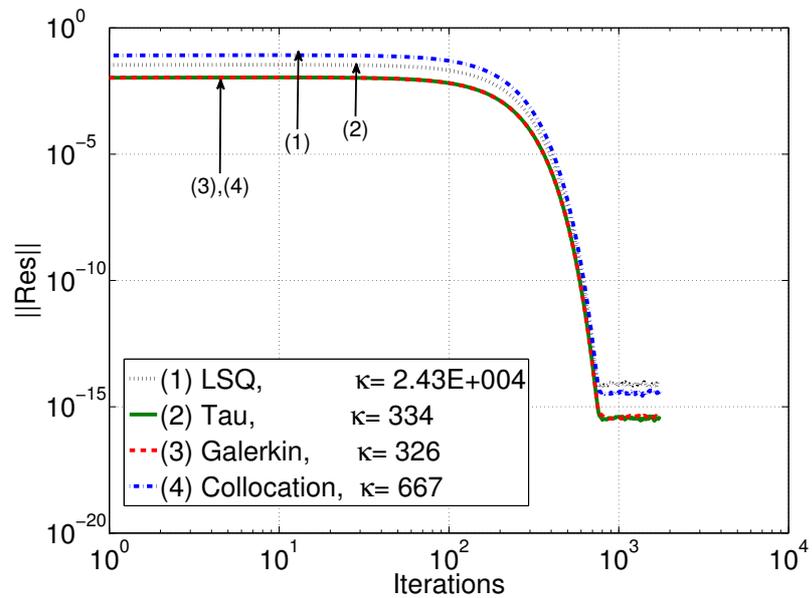


Figure 3: Convergence plot and condition number κ . Methanol synthesis. $N = 10$.

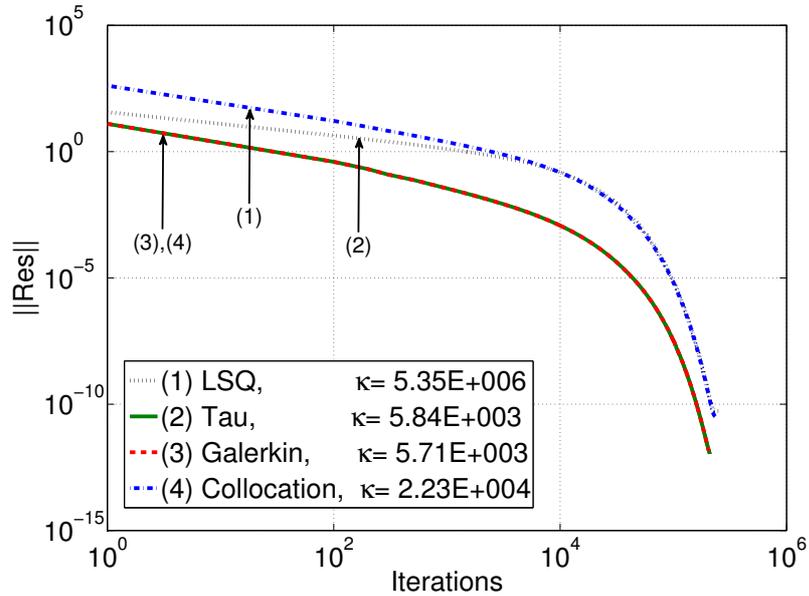


Figure 4: Convergence plot and condition number κ . SMR process. $N = 40$.

6 Conclusion

A non-linear pellet model has been solved for the SMR process and methanol synthesis using the orthogonal collocation, Galerkin, tau and least-squares methods. Considering the accuracy of the numerical techniques, the Galerkin and tau methods are recommended above the orthogonal collocation and least-squares methods. Considering implementation issues, the orthogonal collocation is associated with less theoretical complexities, whereas the Galerkin is considered the most time consuming method to implement.

The evaluation of the weighted residual methods should be further analysed on other type of differential equations adopted in chemical reactor engineering.

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Notation list

Latin Letters

a	Matrix coefficient element
A	Coefficient matrix
\mathcal{B}	Boundary operator
B	Permeability (m^2)
C_p	Heat capacity (J/kmol/K)
\tilde{C}_p	Heat capacity (J/kg/K)
D_{ij}	Binary diffusion coefficient (m^2/s)
d_{pore}	Pore diameter (m)
d	Diameter of pellet (m)
f	Unknown function
F	Source vector
g	Source vector
ΔH	Heat of reaction (J/kmol)
j	Mass diffusion flux ($\text{kg/m}^2/\text{s}$)
\mathcal{J}	Functional
ℓ	Lagrange polynomial
\mathcal{L}	Linear operator
M	Molecular weight (kg/kmol)
MeOH	Methanol
n	Number of species in the gas mixture
N	Number of collocation/quadrature points
p	Pressure (Pa)
r_p	Radius of pellet (m)
r	Radial dimension (m)
R	Gas constant (J/kmol/K)
Res	Residual
\mathcal{R}	Residual
\tilde{S}_i	Mass source term of species i ($\text{kg/m}^3/\text{s}$)
S	Heat source term ($\text{J/m}^3/\text{s}$)
SMR	Steam methane reforming
t	Time (s)
T	Temperature (K)
v	Mass average velocity (m/s)
v	Perturbation function; variational analysis
W	Quadrature weight
Q	Heat flux ($\text{J/m}^2/\text{s}$)
x	Coordinate (m)
$\mathcal{X}(\Omega)$	Space
$\mathcal{X}^s(\Omega)$	Trial function space

Greek Letters

α	Basis coefficient
α	Under-relaxation factor
λ	Conductivity (W/m/K)
ρ	Density (kg/m ³)
ω	Mass fraction (-)
μ	Viscosity (kg/m/s)
Ω	Computational domain
ϵ	Void fraction (-)
τ	Tortuosity (-)
Γ	Boundary
φ	Basis or trial function
ϵ	Amplitude variable; variational analysis
δ	Dirac delta function
ψ	Weighting function

Subscript

b	Bulk
g	Gas
p	Pellet
i_q	Quadrature point
i	Species type
j	Species type
j	Index associated with polynomial order
i	Index associated with the points
Γ	Boundary

Superscript

e	Effective
s	Superficial
T	Transpose
P	Polynomial order